Complexity of
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on Structures of Bounded Degree

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Abstract

Normal forms express semantic properties of logics by means of syntactical restrictions. Often, normal forms allow algorithms to benefit from restrictions of the expressive power of a logic. A typical example is the locality of first-order logic (FO), which implies that, e.g., properties like reachability or connectivity cannot be defined in FO. This is formalised by Gaifman's local normal form, which states the satisfaction conditions of an FO-formula by a Boolean combination of local statements. Gaifman normal form serves as a first step in fixed-parameter model-checking algorithms, parameterised by the size of the formula, on a wide range of sparse graph classes. However, it is known that, even on acyclic graphs, there are non-elementary lower bounds for the costs involved in transforming a formula into Gaifman normal form. This leads to an enormous parameter-dependency of the aforementioned algorithms. Similar non-elementary lower bounds also hold for Feferman-Vaught decompositions, which are an important tool in model-checking and satisfiability-checking, and for the preservation theorems by Lyndon, Łoś, and Tarski, stating that a formula is preserved under extensions (homomorphisms) if and only if it is equivalent to an existential (existential-positive) formula.

This thesis investigates the complexity of these normal forms when restricting attention to classes of structures of bounded degree, for which the non-elementary lower bounds are known to fail. As a matter of fact, the thesis provides algorithms with elementary and even worst-case optimal running time for the construction of Gaifman normal form and Feferman-Vaught decompositions under this restriction. For the preservation theorems, algorithmic versions with elementary running time and non-matching lower bounds are provided.

Crucial for these results is the notion of Hanf normal form, which, on classes of structures of bounded degree, is also in its own right an important ingredient for algorithms. Here, the present thesis provides a characterisation of sets of unary counting quantifiers in terms of ultimately periodic sets, for which the respective extensions of FO allow generalisations of Hanf normal form. In particular, this includes modulo-counting quantifiers. For all such extensions, a construction of Hanf normal form with worst-case optimal running time is presented. On classes of structures of bounded degree, this leads to fixed-parameter model-checking algorithms for all such extensions and also allows respective generalisations of the constructions for Feferman-Vaught decompositions and preservation theorems.

Zusammenfassung

Normalformen drücken semantische Eigenschaften einer Logik durch syntaktische Restriktionen aus. Sie ermöglichen es Algorithmen, Grenzen der Ausdrucksstärke einer Logik auszunutzen. Ein Beispiel ist die Lokalität der Logik erster Stufe (FO), die impliziert, dass Graph-Eigenschaften wie Erreichbarkeit oder Zusammenhang nicht FO-definierbar sind. Gaifman-Normalformen drücken die Bedeutung einer FO-Formel als Boolesche Kombination lokaler Eigenschaften aus. Sie haben eine wichtige Rolle in Model-Checking Algorithmen für eine Vielzahl von Klassen dünn besetzter („sparse") Graphen, deren Laufzeit durch die Größe der auszuwertenden Formel parametrisiert ist. Selbst für Klassen azyklischer Graphen ist jedoch bekannt, dass Gaifman-Normalformen nur mit nicht-elementarem Aufwand konstruiert werden können. Dies führt zu einer enormen Parameterabhängigkeit der genannten Algorithmen. Ähnliche nicht-elementare untere Schranken sind auch für Feferman-Vaught-Zerlegungen bekannt, die ein wichtiges Werkzeug für Model-Checking und Erfüllbarkeitsalgorithmen sind, und für die Erhaltungssätze von Lyndon, Łoś und Tarski, laut denen die Gültigkeit einer Formel unter Erweiterungen (Homomorphismen) genau dann erhalten bleibt, wenn die Formel zu einer existenziellen (existenziell-positiven) Formel äquivalent ist.

Diese Arbeit untersucht die Komplexität der genannten Normalformen auf Klassen von Strukturen beschränkten Grades, für welche die nicht-elementaren unteren Schranken nicht gelten. Für diese Einschränkung werden Algorithmen mit elementarer Laufzeitschranke für die Konstruktion von Gaifman-Normalformen, Feferman-Vaught-Zerlegungen, und für die Erhaltungssätze von Lyndon, Łoś und Tarski, vorgestellt, die in den ersten beiden Fällen sogar worst-case optimal sind.

Ein wichtiges Werkzeug hierfür sind Hanf-Normalformen die, auf Klassen von Strukturen beschränkten Grades, auch Anwendungen in Algorithmen finden. Ein weiterer Beitrag dieser Arbeit ist eine Charakterisierung von Mengen unärer Zählquantoren, für die die jeweilige Erweiterung von FO Hanf-Normalformen erlaubt. Es stellt sich heraus, dass dies genau die Zählquantoren sind, die durch ultimativ-periodische Mengen charakterisiert sind. Dies schließt insbesondere Modulo-Zählquantoren ein. Für Erweiterungen von FO durch solche ultimativ-periodische Zählquantoren wird eine worst-case optimale Konstruktion von Hanf-Normalformen beschrieben. Auf Klassen von Strukturen von beschränktem Grad führt dies für solche Erweiterungen von FO zu parametrisierten Model-Checking-Algorithmen und zu Verallgemeinerungen der Algorithmen für Feferman-Vaught-Zerlegungen und die Erhaltungssätze von Lyndon, Łoś und Tarski.

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In memory of Michael Härtel
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Contents

1 Introduction

Normal forms express semantic properties of a logic by means of syntactical restrictions. On the one hand, this can be used for inexpressibility results, that is, for showing that certain properties are not definable in the logic (cf., e.g., [Lib97, LN00, EF99, Lib04]). On the other hand, normal forms make limitations of the expressive power of a logic accessible for algorithmic purposes [See96, FG01, GW04, FG04, Kre11, GKS14, DG07, KS11, DSS14, Seg14, BKS17, KS17].

In particular in the latter context, not only the existence of normal forms is of interest, but also their *efficiency*, that is, the size of the normal form in comparison to the original formula, and the resources required for its construction [GW04, DGKS07, DG07, Lin08, BK12, HKS13, HKS16, KS17].

A typical example is *Gaifman normal form* [Gai82] for first-order logic, which makes local conditions for the validity of a formula in a structure explicit. On various classes of sparse structures, Gaifman normal form leads to fixed-parameter tractable model-checking algorithms that are parameterised by the size of the input formula [FG01, GW04, FG04, Kre11, GKS14]. More precisely, the algorithm's running time only depends linearly or pseudo-linearly on the size of the structure the input formula is checked against. On the other hand, the running time in terms of the size of the input formula depends on the time needed for turning the formula into Gaifman normal form.

However, it was shown that, without further restrictions, this transformation is only possible with non-elementary cost [DGKS07]. Thus, the parameter-dependency of such a model-checking algorithm is not bounded by any k-fold exponential function for any $k \in \mathbb{N}$ whatsoever.

Similar lower bounds were shown for the size of *Feferman-Vaught decompositions* [DGKS07] and for the *preservation theorems of Lyndon, Łoś, and Tarski*. More precisely, there are non-elementary lower bounds on the size of an equivalent *existential sentence* for a sentence that is preserved under extensions [DGKS07], and for the size of an equivalent *existential-positive sentence* for a sentence that is preserved under homomorphisms [Gur90, Ros08].

A closer look at the lower bound proofs shows their failure on *classes of* *structures of bounded degree.* A structure has degree $\leq d$ (for some $d \in \mathbb{N}$) if for each of its elements, there are at most d other elements with which it occurs together in the tuples of the relations of the structure. A class of structures has bounded degree if there is a $d \in \mathbb{N}$ such that all structures in the class have degree $\leq d$.

This thesis provides an analysis of the efficiency of the mentioned normal forms when equivalence to the original formulae is only required with respect to a class of structures of bounded degree. Under this relaxation, *algorithms with elementary running time* are developed and complemented by – mostly – *matching lower bounds* [HKS13, HHS14, HHS15].

For classes of structures of bounded degree, crucial tools for the above mentioned results are Hanf's locality theorem [Han65, FSV95] for first-order logic and the corresponding *Hanf normal form* [EF99, BK12]. Both also found important applications in algorithms on classes of structures of bounded degree in their own right [See96, FG04, DG07, KS11, BKS17, KS17].

Hanf's locality theorem does not only hold for first-order logic but has a generalisation to the extension of first-order logic by modulo-counting quantifiers [Nur00], which also gives rise to a normal form [HKS16]. This motivates a second line of results of this thesis, examining extensions of first-order logic by *unary counting quantifiers.* Here, a complete characterisation of all the sets of unary counting quantifiers that have an analogue to Hanf's theorem and Hanf normal form is given in terms of *ultimately periodic sets* (cf. [Mat94]). Furthermore, it is shown that in all these cases, the corresponding variant of Hanf normal form can be computed in worst-case optimal time [HKS16].

The generalisation of Hanf normal form to formulae using ultimately periodic quantifiers also leads to corresponding generalisations of the elementary algorithms concerning Feferman-Vaught decompositions and preservation theorems.

A well-known construction (cf., e.g., [Str94]), which resolves tuple-counting quantifiers into quantifiers counting only single elements of structures, furthermore allows to extend these results to ultimately periodic tuple-counting quantifiers.

The results presented in this thesis were largely already published in [HKS13, HHS14, HHS15, HKS16]. In the following pages, an overview over these results is given. To this aim, the normal forms of concern are informally introduced and previous work, in particular with a focus on applications of the normal forms and known upper and lower bounds for their efficiency, is mentioned. The overview is in parts based on [HKS13, HHS14, HHS15, HKS16].

Normal Forms for Locality

It is known that first-order logic[1] (FO) can only express local properties (cf., e.g., [Han65, Gai82, FSV95, SB99, EF99, Lib04]). In particular, this excludes properties like connectivity or reachability in graphs, which can only be decided by a global view on the graph (cf., e.g., [FSV95, EF99, Lib04]). There are different formalisations of this limitation to the expressive power of FO in the shape of theorems by Hanf, by Gaifman, and by Schwentick and Barthelmann [Han65, Gai82, FSV95, SB99]. All these formalisations of locality give rise to normal forms for FO.

In particular, sentences in Hanf normal form [EF99, BK12] are Boolean combinations of statements of the form

(H) *"there are $\geq k$ elements whose r-neighbourhood has isomorphism type τ",*

whereas sentences in Gaifman normal form [Gai82] are Boolean combinations of statements of the form

(G) *"there are $\geq k$ elements x of pairwise distance $> 2r$ whose r-neighbourhood satisfies a formula $\varrho(x)$."*

For formulae with free variables, Hanf normal form additionally allows statements that check the isomorphism type of the r-neighbourhood of their free variables [HKS16]. For the same purpose, Gaifman normal form uses, more generally, formulae whose validity only depends on the r-neighbourhood of their free variables [Gai82].

An important difference between Hanf's and Gaifman's theorem is that the former only applies to classes of structures of bounded degree, while the latter applies to all relational structures.

The theorems of Hanf and Gaifman have found various applications in algorithms and complexity (cf., [See96, LN00, Lib97, FG01, GW04, DGKS06, DG07, Kre11]). In particular, there are very general algorithmic meta-theorems stating that FO model-checking is fixed-parameter tractable for various classes of sparse structures, ranging from classes of structures of bounded degree to

[1] In the subsequent chapters of this thesis, threshold-counting quantifiers, stating that there are $\geq k$ witnesses for a quantified formula, are often assumed to be built-in. However, they can easily be expressed in plain first-order logic with a slight increase in quantifier rank and formula size. For the introduction, we can ignore this distinction.

classes that are nowhere dense [See96, FG01, GW04, FG04, Kre11, GKS14]. Furthermore, it was proven that results of queries defined by formulae of FO (and certain extensions of it) on classes of structures of bounded degree or low degree can be enumerated with constant delay after a (pseudo-)linear time preprocessing phase [DG07, KS11, DSS14, Seg14, BKS17, KS17]. Another application are polynomial time approximation schemes for FO-definable optimisation problems on classes with excluded minors [DGKS06]. In the context of such applications, the efficiency of constructing such normal forms has attracted interest [GW04, DGKS07, DG07, Lin08, BK12, HKS13, HKS16, KS17].

Hanf Normal Form

A direct consequence of Hanf's locality theorem [Han65, FSV95] is that for each FO-formula φ over a relational signature σ, and for every degree bound $d \geq 0$, there exists a d-equivalent Hanf normal form ψ, that is, a Hanf normal form which is equivalent to φ on all σ-structures of degree $\leq d$ [EF99, BK12].

A first algorithm for the construction of such Hanf normal form for FO was described in [See96]. However, this algorithm is not primitive-recursive. The first primitive-recursive algorithms for computing Hanf normal form can be found in [DG07, Lin08]. The algorithm from [DG07], at first sight, seems to be non-elementary, but it actually is 4-fold exponential [Clo12, HKS13]. Finally, a 3-fold exponential algorithm and a matching lower bound were presented in [BK12].

Modulo-Counting Quantifiers

Notions of locality have also been developed for extensions of FO, and they have found application in proving inexpressibility results for these logics (cf., e.g., [Nur96, Lib98, HLN99, Nur00, LN00, Lib04, KS17]). When restricting attention to classes of finite structures of bounded degree, these locality notions also give rise to normal forms for the respective logics.

In particular, in [Nur00], Nurmonen extended Hanf's locality theorem to the extension of FO by a modulo-counting quantifier D_p of period $p \geq 2$, where a formula of the form $\mathsf{D}_p y\, \psi(\overline{x}, y)$ states that the number of witnesses y for $\psi(\overline{x}, y)$ is divisible by p. As an easy consequence of Nurmonen's theorem, one obtains that for every sentence φ, possibly using the quantifier D_p, and for every degree bound $d \geq 0$, there exists a d-equivalent Boolean combination of statements of the form (H) and of the form

> *"the number of elements whose r-neighbourhood has isomorphism type τ is divisible by p with remainder m."*

Again, we say that ψ is in Hanf normal form.

For algorithmic applications, an effective procedure for computing ψ on input of φ and the degree bound d would be desirable (cf., e.g., the use of Nurmonen's theorem in the proof of Theorem 7 in the full version of [NSST15]). Similarly to Hanf's theorem, the proof of [Nur00], however, does not lead to such an effective procedure.

In this direction, the contribution of this thesis is an algorithm which, on input of a degree bound d and a formula φ from FO extended by an arbitrary set of modulo-counting quantifiers, computes a d-equivalent Hanf normal form. This algorithm uses 3-fold exponential time for $d \geq 3$ and 2-fold exponential time for $d = 2$ and is worst-case optimal in both cases.

As an easy application of this result, we obtain that Seese's [See96] fixed-parameter tractability result for the data complexity of FO model-checking on classes of structures of bounded degree can be generalised to extensions of FO by sets of modulo-counting quantifiers. Moreover, the existence of Hanf normal form for FO with sets of modulo-counting quantifiers also leads to an alternative proof of Nurmonen's locality theorem.

Both aforementioned results were published in [HKS16].

Recently, the construction of Hanf normal form for FO with modulo-counting quantifiers found use in [BKS17]. There, it serves as an intermediate step in algorithms that enumerate the results of queries with constant delay after a linear time preprocessing phase, even in the presence of updates on the database.

Ultimately Periodic Quantifiers

Generalising on Nurmonen's locality theorem and the corresponding Hanf normal form, the following questions arise:

(1) Which extensions of FO by a set C of unary counting quantifiers permit Hanf normal form?

(2) If such an extension of FO permits Hanf normal form, (how) can these Hanf normal forms be computed?

On finite structures, a unary counting quantifier is a subset Q of the natural numbers, and a sentence in Hanf normal form is a Boolean combination of statements of the form

> *"there are $n + k$ elements whose r-neighbourhood has isomorphism type τ, for some number $n \in \mathsf{Q}$"*,

where Q is a quantifier from C or the existential quantifier. We say that the extension of FO by the unary counting quantifiers from the set C permits Hanf normal form if for each relational signature σ and every degree bound d, each formula over the signature σ has a d-equivalent Hanf normal form.

This thesis provides a complete answer to both questions. Concerning Question (1), a characterisation is given to the effect that an extension of FO by unary counting quantifiers permits Hanf normal form if and only if all allowed quantifiers are ultimately periodic. Intuitively, ultimately periodic [Mat94] quantifiers are the quantifiers that can be obtained from Boolean combinations of modulo-counting and threshold-counting quantifiers. Answering Question (2) it is shown that for each such extension of FO, Hanf normal form can also be computed in roughly the same time as for the special case of modulo-counting quantifiers. This way, we also obtain a corresponding generalisation of Seese's model-checking algorithm for ultimately periodic quantifiers. The results presented above were published in [HKS16].

Gaifman Normal Form

Already Gaifman's article [Gai82] provides an algorithm for transforming FO-formulae into Gaifman normal form, which proceeds by an induction over the shape of the input formula. However, this algorithm leads to a non-elementary blow-up of the size of the Gaifman normal form in terms of the quantifier rank of the input formula. In [DGKS07] it is proven that indeed this transformation is only possible at non-elementary cost, if the algorithm has to handle arbitrary FO-formulae and has to return a Gaifman normal form that is equivalent to the input formula on all structures (more generally, even on all finite trees). However, this does not rule out more efficient algorithms (in particular, with elementary running time) for cases where restrictions on the form of the input formula are imposed, or where equivalence of the computed Gaifman normal form to the input formula is only required on a restricted class of structures.

Towards restricted formulae, we know from [GW04] that purely existential formulae can be transformed in 1-fold exponential time into asymmetric Gaifman normal form, which is a slightly weaker variant of Gaifman normal form. Considering fragments of FO with a fixed number of variables, [GJL12] shows that a non-elementary lower bound already holds for the 3-variable fragment of FO.

However, for the 2-variable fragment of FO, [GJL12] describes a transformation into Gaifman normal form that can be carried out in 2-fold exponential time.

Towards restricted classes of structures, a closer look at the proof of the non-elementary lower bound of [DGKS07] shows that the proof fails when restricting attention to a class of graphs of bounded degree. Indeed, [DGKS07] observes that for every FO-formula φ and every degree bound d, there exists a formula in Gaifman normal form that is d-equivalent to φ and whose size is at most 4-fold exponential in the size of φ. The corresponding proof, however, adapts the model theoretic proof of Gaifman's theorem presented in [EF99], and does not lead to a primitive-recursive algorithm. The first procedure with elementary (in fact, 5-fold exponential) running time is based on the algorithm of [Gai82] and was developed in the author's master's thesis [Hei12].

The contribution of this thesis is an algorithm which, on input of a degree bound d and an FO-formula φ, computes a d-equivalent Gaifman normal form. For $d \geq 3$, the algorithm takes 3-fold exponential time in the size of φ, and for $d = 2$, it takes 2-fold exponential time. For both cases, the algorithm is shown to be worst-case optimal (for binary trees, that is, degree bound 3, this was already proven in [Hei12]).

The results presented in this section are published in [HKS13].

Feferman-Vaught Decompositions

The theory of a structure is the set of FO-sentences that hold in this structure [Hod93]. The classical Feferman-Vaught theorem [FV59] states that for certain forms of compositions of structures, the theory of a structure composed from component structures is determined by the theories of the component structures. Compositions for which this applies are, for example, disjoint unions and, more generally, disjoint sums, as well as direct products[2] (cf., e.g., [Hod93]). Feferman-Vaught like theorems find application in results concerning the decidability of theories, as well as for model-checking and satisfiability-checking (cf., e.g., [Mak04, GJL12]). Regarding first-order logic, another important application lies within the proof of Gaifman's theorem [Gai82].

Another way to express decompositions à la Feferman-Vaught, which is particularly useful for algorithmic applications, uses so-called reduction sequences [FV59, Mak04, GJL12]: A given sentence φ that shall be evaluated

[2] also known as cartesian products or as tensor products

in the composition $\mathcal{A}$ of s structures $\mathcal{A}_1, \dots, \mathcal{A}_s$, can be transformed into a sequence $\Delta_1, \dots, \Delta_s$ of finite sets of formulae and a propositional formula β whose propositions are tests of the form

"the i-th structure $\mathcal{A}_i$ satisfies the j-th formula in the i-th set Δ_i",

such that $\mathcal{A}$ is a model of φ if and only if β is true.

One way to compute such a decomposition is via quantifier elimination (cf., e.g., [Mak04]). Such a quantifier elimination preserves the quantifier rank of the input formula. That is, if φ has quantifier rank q, then also the formulae in the sets $\Delta_1, \dots, \Delta_s$ have quantifier rank at most q. On the other hand, a similar correspondence does not hold for formula size. In [DGKS07] it was shown that a non-elementary blow-up of the decomposition is unavoidable, even when only trees are considered as component structures. However, this does not rule out better (in particular, elementary) upper bounds when restricting the shape of the input formula to be decomposed, or when imposing restrictions to the component structures considered.

Towards restricted formulae, [GJL12] shows that a non-elementary lower bound already holds for the 3-variable fragment of FO, whereas for the 2-variable fragment, a 2-fold exponential upper bound can be shown.

Towards restricted classes of component structures, the present thesis contributes an algorithm which, on input of an FO-formula with ultimately periodic quantifiers, and an arity $s \geq 1$, computes a decomposition with respect to disjoint sums of relational structures of degree at most d. For degree bounds $d \geq 3$, the algorithm has 3-fold exponential time complexity and, for $d = 2$, 2-fold exponential time complexity. For both cases, it is furthermore shown to be worst-case optimal. Note that, as with Hanf normal form, ultimately periodic quantifiers turn out to be the largest class of unary counting quantifiers where every formula using these quantifiers is guaranteed to have a decomposition with respect to disjoint sums.

Regarding other forms of compositions, the algorithm is generalised to decompositions with respect to compositions obtained by applying transductions to disjoint sums. As a particular example, this leads to an algorithm with roughly the same time complexity for the construction of decompositions with respect to direct products of d-bounded structures.

For the case of input formulae from FO, the algorithms for decompositions with respect to disjoint sums, direct products, and transductions over disjoint sums, as well as the corresponding lower bound were published in [HHS14, HHS15].

Preservation Theorems

Preservation theorems are classical results of model theory that relate syntactic restrictions of formulae with structural properties of the classes of structures defined by the formulae (cf., e.g., [Lyn59, Hod93]). They are originally proven using the compactness theorem for first-order logic [Lyn59, Hod93] and thus are stated for the class of all (that is, finite and infinite) structures. In the following, we let σ be a relational signature and denote by $\mathfrak{C}$ the class of all, finite and infinite, structures over this signature. Furthermore, we only consider formulae over the signature σ.

The Łoś-Tarski theorem (cf., e.g., [Hod93]) states the following equivalence for each FO-sentence φ:

φ is preserved under extensions on $\mathfrak{C}$

iff φ is equivalent to an existential sentence on $\mathfrak{C}$.

Here, φ is said to be preserved under extensions on $\mathfrak{C}$ if every structure in $\mathfrak{C}$ that contains a model of φ from $\mathfrak{C}$ as an induced substructure is also a model of φ. Furthermore, a formula is existential if it is quantifier-free, apart from a prefix of existential quantifiers.

On the other hand, the homomorphism preservation theorem (also called Lyndon-Łoś-Tarski theorem, cf., e.g., [Lyn59, Hod93, Ros08]) states that an FO-sentence

φ is preserved under homomorphisms on $\mathfrak{C}$

iff φ is equivalent to an existential-positive sentence on $\mathfrak{C}$.

Here, φ is said to be preserved under homomorphisms on $\mathfrak{C}$ if for any two structures $\mathcal{A}, \mathcal{B} \in \mathfrak{C}$, if $\mathcal{A}$ is a model of φ and there is a homomorphism from $\mathcal{A}$ to $\mathcal{B}$, then also $\mathcal{B}$ is a model of φ. Furthermore, a formula is existential-positive if it is existential and the quantifier-free subformula is only built from atomic formulae as well as conjunctions and disjunctions. In the context of database theory, existential-positive formulae correspond to unions of conjunctive queries, which are a typical and, in practice, very common class of database queries [AHV95].

Since, in both preservation theorems, the class $\mathfrak{C}$ occurs in the hypothesis as well as in the conclusion of the biimplication, neither the Łoś-Tarski theorem nor the homomorphism preservation theorem relativise straightforwardly to restricted classes of structures, e.g., to the class of finite structures.

Indeed, it turned out that the Łoś-Tarski Theorem fails when considering the class of all finite structures instead of the class of all finite and infinite structures [Tai59, Gur84]. On the other hand, in [ADG08] it was shown to hold for various classes of structures, including the class of all finite structures of degree at most d, the class of all finite structures of treewidth at most k, and all wide classes of structures that are closed under taking substructures and disjoint unions.

The homomorphism preservation theorem was shown to hold on the class of all finite structures [Ros08, Ros16], as well as for the classes of all finite structures of degree at most d or of treewidth at most k [ADK06], and, in general, for quasi-wide classes of structures that are closed under taking substructures and disjoint unions [Daw10], which includes classes of bounded expansion and classes that locally exclude minors.

For classes of structures for which a theorem in the style of the Łoś-Tarski theorem or the homomorphism preservation theorem is known to hold, it is of interest to understand the complexity of the construction of an existential or existential-positive sentence, given a sentence that is preserved under extensions or homomorphisms on the class, respectively.

Preservation under Extensions

In [DGKS07], a lower bound in respect to a class of finite acyclic structures is shown, where sentences that are preserved under extensions on this class have non-elementarily larger existential sentences. For another class of finite structures, even a non-recursive lower bound is known (Benjamin Rossman, personal communication, 2nd Decembre, 2013). However, the proofs of these lower bounds fail on classes of structures of bounded degree. For this case, a 5-fold exponential upper bound on the size of existential sentences for the class of *acyclic* structures of degree at most d was shown in [DGKS07].

The present thesis generalises this result in the following ways:

(1) It is shown that the 5-fold exponential upper bound of [DGKS07] holds for *every* class of structures of degree at most d that is closed under taking induced substructures and disjoint unions.

(2) The existential sentences do not only have at most 5-fold (3-fold) exponential size in terms of the size of the input sentence, but can also be computed within 5-fold (3-fold) exponential time for degree bounds $d \geq 3$ ($d = 2$).

(3) The algorithm does not only allow input sentences from FO, but formulae with free variables that may also use ultimately periodic quantifiers.

The main ingredient of the proof is a new upper bound on the size of minimal models of formulae that are preserved under extensions on the respective class. This upper bound is based on an iterative construction using Hanf's theorem.

The 5-fold exponential upper bound is complemented by a non-matching 3-fold exponential lower bound.

For the case of input sentences from FO extended by a modulo-counting quantifier, the algorithm and the lower bound were published in [HHS14, HHS15].

Preservation under Homomorphisms

Similarly to preservation under extensions, it is shown in [Gur90, Ros08] that there is a class of finite acyclic structures where the construction of existential-positive sentences for sentences that are preserved under homomorphisms on this class leads to a non-elementary blow-up of the formula size.

In contrast, for any class of structures of degree at most d that is closed under taking induced substructures and disjoint unions, and that is decidable in 1-fold exponential time (this is the case, e.g., for the class of all finite structures of degree at most d), the present thesis contributes an algorithmic version of the homomorphism preservation theorem on this class. As input, the algorithm takes a formula from the extension of first-order logic by ultimately periodic quantifiers, which is preserved under homomorphisms on the respective class, and it outputs an existential-positive FO-formula that is equivalent to the input formula on this class. For degree bounds $d \geq 3$, this takes 4-fold exponential time, and it takes 3-fold exponential time for $d = 2$.

The 4-fold exponential upper bound is complemented by a non-matching 3-fold exponential lower bound.

For the case of input sentences from FO extended by a modulo-counting quantifier, the algorithm and the lower bound were published in [HHS14, HHS15].

About the Thesis

This section gives an overview over the publications this thesis is based on. The publications are co-authored with Frederik Harwath, Dietrich Kuske, and Nicole Schweikardt, and presented in chronological order.

[HKS13] Lucas Heimberg, Dietrich Kuske, and Nicole Schweikardt. An optimal Gaifman normal form construction for structures of bounded degree. In *Proceedings of the 28th Annual ACM/IEEE Symposium on Logic in Computer Science, (LICS 2013)*, pages 63–72, 2013.

The algorithm for the construction of Gaifman normal form of [HKS13] is presented in Chapter 4, where it is very slightly extended to FO with threshold-counting quantifiers. The corresponding lower bound of [HKS13] is presented in Section 9.4, where it is strengthened to a sequence of lower bounds for growing degree bounds.

[HHS14] Frederik Harwath, Lucas Heimberg, and Nicole Schweikardt. Preservation and decomposition theorems for bounded degree structures. In *Joint Meeting of the 23rd EACSL Annual Conference on Computer Science Logic (CSL) and the 29th Annual ACM/IEEE Symposium on Logic in Computer Science (LICS), (CSL-LICS 2014)*, pages 49:1-49:10. ACM, 2014.

[HHS15] Frederik Harwath, Lucas Heimberg, and Nicole Schweikardt. Preservation and decomposition theorems for bounded degree structures. *Logical Methods in Computer Science*, 11(4), 2015.

The algorithms for preservation theorems of [HHS14, HHS15], as well as the counterexamples, showing the necessity of closure under disjoint unions and induced substructures for the underlying classes of structures, are presented in Section 6.2, Section 6.3, and Section 6.4, respectively. There, the algorithms are generalised to input formulae with free variables and to extensions of FO by threshold-counting quantifiers and arbitrary sets of modulo-counting quantifiers. In Section 7.5, both algorithms are extended to FO with threshold- and modulo-counting quantifiers that may also count tuples. Finally, Section 8.6 generalises both algorithms to extensions of FO by ultimately periodic tuple-counting quantifiers. The lower bounds concerning preservation under extensions and preservation under homomorphisms of [HHS14, HHS15] are presented in Section 9.6.

The constructions for Feferman-Vaught decompositions of [HHS14, HHS15] are presented in Chapter 5 and, for the case of disjoint sums, generalised to FO with threshold- and modulo-counting quantifiers. In Section 7.4, the algorithms for Feferman-Vaught decompositions with respect to disjoint sums, direct products, and transductions over disjoint sums are lifted to FO with threshold- and modulo-counting quantifiers over tuples. Finally, Section 8.5 generalises all three constructions to FO with ultimately periodic tuple-counting quantifiers. Furthermore, it is shown there, using an idea of [HKS16], that ultimately periodic quantifiers are also the largest set of unary counting quantifiers permitting decompositions with respect to disjoint sums. The lower bound of [HHS14, HHS15] concerning Feferman-Vaught decompositions with respect to disjoint sums is presented in Section 9.5 and strengthened to a sequence of lower bounds for growing degree bounds.

[HKS16] Lucas Heimberg, Dietrich Kuske, and Nicole Schweikardt. Hanf normal form for first-order logic with unary counting quantifiers. In *Proceedings of the 31th Annual ACM/IEEE Symposium on Logic in Computer Science, (LICS 2016)*, pages 63–72, 2016.

The construction of Hanf normal form for first-order logic with modulo-counting quantifiers and a corresponding generalisation of Seese's model-checking algorithm [See96] from [HKS16] are presented in Chapter 3. There, also an alternative proof of Nurmonen's locality theorem [Nur00], based on this Hanf normal form, is presented. In Section 7.3, all these results are generalised to tuple-counting quantifiers. Section 8.3 contains the transformations between modulo-counting and ultimately periodic quantifiers, published in [HKS16]. Section 8.2 and Section 8.4 present the characterisation of sets of unary counting quantifiers that permit Hanf normal form, provided by [HKS16]. Furthermore, Section 8.4 contains the construction of Hanf normal form for ultimately periodic quantifiers and the corresponding generalisation of Seese's model-checking algorithm from [HKS16]. In Chapter 8, the transformations between modulo-counting and ultimately periodic quantifiers of [HKS16] are also used to generalise the algorithms for Feferman-Vaught decompositions and preservation theorems from [HHS14, HHS15] accordingly.

Structure of the Thesis

Chapter 2 introduces basic notations and concepts, as well as a divide-and-conquer scheme for the construction of certain formulae, which will be crucial for the time complexity of the construction of Hanf normal form in Section 3.2, as well as for the construction of existential formulae in Section 6.2 and the transformation of tuple-counting quantifiers in Section 7.2.

Chapter 3 generalises Hanf normal form to extensions of FO by unary counting quantifiers and shows how Hanf normal form for FO with modulo-counting quantifiers can be computed worst-case optimally. The latter result is applied in an alternative proof of Nurmonen's locality theorem and a generalisation of Seese's fixed-parameter model-checking algorithm. The results of this chapter were published in [HKS16].

Chapter 4 computes Gaifman normal form on classes of structures of bounded degree in elementary and, moreover, worst-case optimal time. The results of this chapter were published in [HKS13]

Chapter 5 constructs Feferman-Vaught decompositions for FO-formulae with modulo-counting quantifiers with respect to disjoint sums over classes of structures of bounded degree. For FO-formulae, this is generalised to transductions on disjoint sums and to direct products. For the special case of FO, the results of this chapter were published in [HHS14, HHS15].

Chapter 6 describes elementary algorithms for the construction of existential (existential-positive) formulae for FO-formulae with modulo-counting quantifiers that are preserved under extensions (homomorphisms) on a class of structures of bounded degree that is closed under disjoint unions and induced substructures. It is also shown that these closure properties are unavoidable. The results of this chapter were published in [HHS14, HHS15].

Chapter 7 uses a method from [Str94] to resolve tuple-counting quantifiers into quantifiers that count only single elements. The transformation is described for threshold-counting and modulo-counting quantifiers and generalises the results of Chapter 3, Chapter 5, and Chapter 6.

Chapter 8 transforms between modulo-counting and ultimately periodic quantifiers, which allows a corresponding generalisation of the results presented in Chapter 3, Chapter 5, and Chapter 6 (respectively, their extensions to tuple-quantifiers of Chapter 7). For Hanf normal form and Feferman-Vaught decompositions, it is shown that ultimately periodic quantifiers are the largest class of unary counting quantifiers where this is possible. The transformation between modulo-counting and ultimately periodic quantifiers, as well as the characterisation result for Hanf normal form, are published in [HKS16].

Chapter 9 complements the results of the previous chapters by lower bounds. The lower bounds for Hanf normal form, Gaifman normal form, and Feferman-Vaught decompositions are slight strengthenings of the lower bounds in [BK12, Hei12, HKS13, HHS14, HHS15]. The lower bounds for preservation theorems were published in [HHS14, HHS15].

Chapter 10 concludes the thesis with a summary of its results and mentions some questions left open.

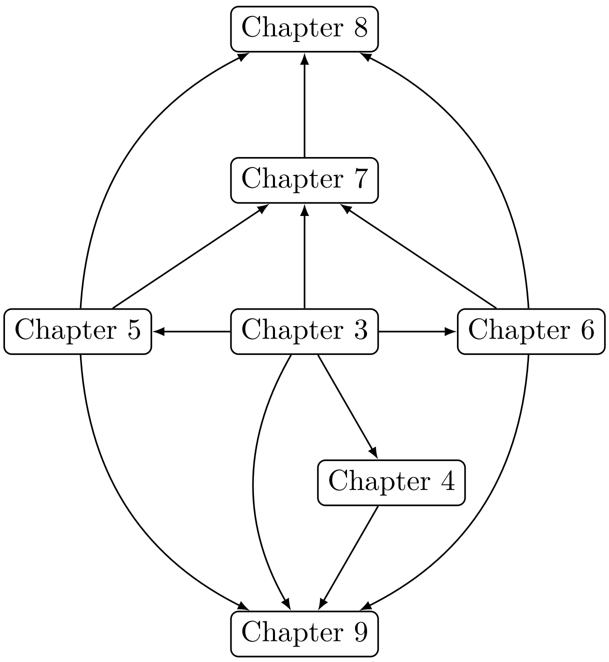

Figure 1.1 Dependencies among the chapters of this thesis

2 Preliminaries

This chapter contains the basic notations and concepts used throughout the thesis. Section 2.1 recalls the essential notation concerning arithmetic and the growth of functions, as well as for finite and infinite words. Section 2.2 shortly discusses the model of computation used for the analysis of algorithms. Section 2.3 introduces finite signatures and finite structures. Section 2.4 defines the logics this thesis is interested in. To this aim, a succession of extensions of first-order logic by unary counting quantifiers is described. Ultimately periodic counting quantifiers will be explained in Section 2.5. Section 2.6 recalls transductions, also called logical interpretations, and states a transduction lemma. In Section 2.7, basic notation about graphs is presented. Section 2.8 recalls the Gaifman graph of structures and uses this concept to define spheres and types – in particular, for classes of structures of bounded degree.

The chapter closes with Section 2.9, where a divide-and-conquer scheme for the construction of formulae will be introduced. This divide-and-conquer scheme will be used later on for a worst-case optimal construction of Hanf normal form in Section 3.2, as well as to improve the time complexity of the construction of existential formulae in Section 6.2 and the transformation of tuple-counting quantifiers in Section 7.2.

2.1 Basic Notation

We write $\mathbb{Z}$ to denote the set of integers and we write $\mathbb{N}$ to denote the set of non-negative integers. For each number $t \in \mathbb{N}$, we let $\mathbb{N}_{\geq t} \coloneqq \{n \in \mathbb{N} : n \geq t\}$. If $n, m \in \mathbb{N}$, then $[n, m]$ denotes the set of all $i \in \mathbb{N}$ with $n \leq i \leq m$. In particular, $[n, m] = \emptyset$ if $m < n$. Furthermore, we let $[n, m) \coloneqq [n, m-1]$.

For a set $M \subseteq \mathbb{N}$, the *least common multiple of the numbers in M* is denoted by $\operatorname{lcm}(M)$. By convention, the least common multiple of an empty set is 1.

For numbers $i, j \in \mathbb{N}$, we let $\operatorname{bit}(j, i) \coloneqq \lfloor i/2^j \rfloor \mod 2$ denote the j-th bit in the binary expansion of i.

Furthermore, we write $\mathbb{R}$ to denote the set of real numbers and we let $\mathbb{R}_{\geq 0}$ denote the set of all non-negative real numbers. For any $r \in \mathbb{R}_{\geq 0}$ with $r > 0$ we write $\log r$ to denote the logarithm of r with respect to base 2.

2.1.1 Growth of Functions

We use the standard $\mathcal{O}$-notation as, e.g., summarised in [FG06, Appendix A]. For a function $f\colon \mathbb{N} \to \mathbb{R}_{\geq 0}$, we write $\mathrm{o}(f)$ to denote the class of all functions $g\colon \mathbb{N} \to \mathbb{R}_{\geq 0}$ where for all $c \in \mathbb{N}_{\geq 1}$ there is an $n_0 \in \mathbb{N}$ such that for all $n \in \mathbb{N}$ with $n > n_0$ we have $g(n) \leq \frac{f(n)}{c}$.

Similarly, $\mathcal{O}(f)$ is the class of all functions $g\colon \mathbb{N} \to \mathbb{R}_{\geq 0}$ where there is a $c \in \mathbb{N}_{\geq 1}$ and an $n_0 \in \mathbb{N}$ such that for all $n \in \mathbb{N}$ with $n > n_0$ we have $g(n) \leq c \cdot f(n)$.

We will sometimes use the fact that if $g \in \mathcal{O}(f)$ for a function $g\colon \mathbb{N} \to \mathbb{R}_{\geq 0}$ and an increasing function $f\colon \mathbb{N} \to (\mathbb{R}_{\geq 0}\setminus\{0\})$, then there is a number $c \in \mathbb{N}_{\geq 1}$ such that $g(n) \leq c \cdot f(n)$ for all $n \in \mathbb{N}$.

Furthermore, we write $\mathrm{poly}(f)$ to denote the class of all functions $g\colon \mathbb{N} \to \mathbb{R}_{\geq 0}$ for which there exists a number $c \in \mathbb{N}_{\geq 1}$ and an $n_0 \in \mathbb{N}$ such that for all $n \in \mathbb{N}$ with $n > n_0$ we have $g(n) \leq (f(n))^c$.

The function $\mathrm{Tower}\colon \mathbb{N} \times \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ is defined by (cf., e.g., [DGKS07])

$$\mathrm{Tower}(0, r) \ \coloneqq \ r \quad \text{and} \quad \mathrm{Tower}(n, r) \ \coloneqq \ 2^{\mathrm{Tower}(n-1,r)}$$

for each $n \geq 1$ and all $r \in \mathbb{R}_{\geq 0}$. That is,

$$\mathrm{Tower}(n, r) \ = \ \left.2^{2^{\cdot^{\cdot^{\cdot^{2^r}}}}}\right\} \text{ a tower of 2s of height } n \text{ with } r \text{ on top.}$$

For $n \in \mathbb{N}$, we abbreviate $\mathrm{Tower}(n) \coloneqq \mathrm{Tower}(n, 1)$.

We say that a function $f\colon \mathbb{N} \to \mathbb{R}_{\geq 0}$ is *at most k-fold exponential*, for some $k \in \mathbb{N}$, if $f(n) \in \mathrm{Tower}(k, \mathrm{poly}(n))$. More generally, f is called *elementary* if it is k-fold exponential for some $k \geq 0$.

2.1.2 Words

Let Σ be a set (which we also call *alphabet*). A *finite word over* Σ is a sequence $w = w_0 w_1 \cdots w_{n-1}$ of *length* $n \geq 0$ of elements from Σ. We also write $|w|$ for the length of w. By ϵ we denote the (unique) *empty word*, that is, the word of length 0. By Σ^* we denote the *set of all finite words over* Σ.

An *ω-word over* Σ (cf., e.g., [Str94]) is a sequence $w = w_0 w_1 w_2 \cdots$ where, for each $n \in \mathbb{N}$, $w_i \in \Sigma$. For each $n \in \mathbb{N}$, we write $w[n]$ to denote the letter w_n in w

at position n, and for numbers $i, j \in \mathbb{N}$ with $i \leq j$, we write $w[i, j]$ for the (finite) word $w_i w_{i+1} \cdots w_j$. Similarly, $w(i, j]$ denotes the (finite) word $w_{i+1} \cdots w_j$. In particular, $w(i, i]$ is the empty word ϵ, and $w(j-1, j] = w[j]$. By Σ^ω we denote the *set of all ω-words over* Σ. We denote the concatenation of a finite word u and a word v (which may be a finite word or an ω-word) by uv. Then, we also call u a *prefix* of uv.

Often, we will also call a finite word a *tuple*. In this context, we write $\overline{a} = (a_1, \ldots, a_n)$ for the word $a_1 \cdots a_n$ of length $n \geq 0$ with $a_1, \ldots, a_n$ from Σ. For each $m \geq 0$ and indices $1 \leq i_1 < \cdots < i_m \leq n$, the tuple $(a_{i_1}, \ldots, a_{i_m})$ is a *subtuple* of $\overline{a}$.

2.2 Model of Computation

We use Random Access Machines as introduced in [FG06, Appendix A.1]: A Random Access Machine (RAM) consists of a *finite control unit*, a *program counter*, and an infinite sequence $r_0, r_1, r_2, \ldots$ of *registers*. Each of these registers stores a natural number. Often, we will also store words over other countable alphabets Σ in sequences of registers. In these cases, we assume some bijection between Σ and a subset of the natural numbers. A program for a RAM consists of a sequence of instructions, indexed by the program counter. Instructions include the arithmetic instructions addition, subtraction, and division by 2, restricted to the natural numbers. Furthermore, there are instructions available for indirect addressing and conditional as well as unconditional jumps.

The input and the output of a RAM are finite words from Σ^* stored in an initial segment of its registers. In order to measure the running time of a RAM we use the *uniform cost measure*, where the time needed for a run of a RAM is measured as the number of instructions carried out and thus, in particular, is independent of the size of the numbers in the registers. A RAM program runs in time $t \colon \mathbb{N} \to \mathbb{N}$ if for every input word $w \in \Sigma^*$, the length of the run of the program on input w is at most $t(|w|)$.

We call an algorithm k-fold exponential for a $k \in \mathbb{N}$, if it can be performed by a RAM program in time t for a k-fold exponential function $t \colon \mathbb{N} \to \mathbb{N}$. More general, we call the algorithm elementary if it is k-fold exponential for some $k \in \mathbb{N}$.

2.3 Signatures and Structures

In this section, we recall notation concerning signatures, structures, and relations between structures, which is based on the standard notation used in, e.g., [EF99, Lib04]. The section also describes encodings for signatures and structures as input for a RAM.

2.3.1 Signatures

By Rel and Const we denote countable sets of *relation symbols* and *constant symbols*, respectively. A function $\mathrm{ar}\colon \mathsf{Rel} \to \mathbb{N}_{\geq 1}$ associates every relation symbol $R \in \mathsf{Rel}$ with its *arity*. A *signature* σ is a tuple $(R_1, \ldots, R_k, c_1, \ldots, c_\ell)$ of $k \geq 0$ distinct relation symbols $R_1, \ldots, R_k \in \mathsf{Rel}$ and $\ell \geq 0$ distinct constant symbols $c_1, \ldots, c_\ell \in \mathsf{Const}$. The signature σ is called *relational* if $\ell = 0$, that is, if it only contains relation symbols.

We represent σ as a finite word over the alphabet $\mathsf{Rel} \cup \mathsf{Const} \cup \{\#\}$. More precisely, we let

$$\mathrm{rep}(\sigma) \ \coloneqq \quad R_1^{\mathrm{ar}(R_1)} \cdots R_k^{\mathrm{ar}(R_k)} \# c_1 \cdots c_\ell.$$

The *size* $||\sigma||$ of a signature σ is the length of $\mathrm{rep}(\sigma)$. Note that, in particular, $||\sigma|| = \ell + 1 + \sum_{i=1}^{k} \mathrm{ar}(R_i)$, that is, the number of its constant symbols plus the sum of the arities of its relation symbols.

2.3.2 Structures

A σ-*structure* $\mathcal{A}$ is a tuple $(A, R_1^{\mathcal{A}}, \ldots, R_k^{\mathcal{A}}, c_1^{\mathcal{A}}, \ldots, c_\ell^{\mathcal{A}})$ consisting of a *finite* non-empty set A, also called the *universe* of $\mathcal{A}$, a relation $R_i^{\mathcal{A}} \subseteq A^{\mathrm{ar}(R_i)}$ for each $i \in [1, k]$, and an element $c_i^{\mathcal{A}} \in A$ for each $i \in [1, \ell]$.

Suppose that $A = \{a_1, \ldots, a_n\}$ for an $n \geq 1$. Furthermore, suppose that the elements $a_1, \ldots, a_n$ are ordered, e.g., by the linear order on the natural numbers if $A \subseteq \mathbb{N}$ or an ordering provided by the representation of A as natural numbers stored in the registers of a RAM. We represent any relation $R^{\mathcal{A}}$ of $\mathcal{A}$ by the word $\mathrm{rep}(R^{\mathcal{A}}) \coloneqq \overline{a}_1 \cdots \overline{a}_m$, where $\overline{a}_1, \ldots, \overline{a}_m$ are the $m \geq 0$ tuples belonging to the set $R^{\mathcal{A}}$ in their lexicographic order. This way, we can represent $\mathcal{A}$ as a word $\mathrm{rep}(\mathcal{A})$ over the alphabet $A \cup \{\#\}$, defined by

$$\mathrm{rep}(\mathcal{A}) \ \coloneqq \quad a_1 \cdots a_n \# \,\mathrm{rep}(R_1^{\mathcal{A}}) \# \cdots \mathrm{rep}(R_k^{\mathcal{A}}) \# c_1^{\mathcal{A}} \cdots c_\ell^{\mathcal{A}}.$$

The *size* $||\mathcal{A}||$ of a σ-structure $\mathcal{A}$ is defined as the size of its representation, and thus

$$||\mathcal{A}|| \quad = \quad |A| \ + \ \sum_{i=1}^{k}\Big(1 + |R_i^{\mathcal{A}}| \cdot \mathrm{ar}(R_i)\Big) \ + \ 1 \ + \ \ell.$$

In particular, $||\mathcal{A}|| \in \mathcal{O}(||\sigma||) \cdot |A|^{||\sigma||}$.

2.3.3 Relations between Structures

If τ is a subtuple of σ, then for any σ-structure $\mathcal{A}$ we denote by $\mathcal{A}_{|\tau}$ the *τ-reduct* of $\mathcal{A}$, that is, the τ-structure with universe A where $R^{\mathcal{A}_{|\tau}} := R^{\mathcal{A}}$ for each relation symbol R in τ, and where $c^{\mathcal{A}_{|\tau}} := c^{\mathcal{A}}$ for each constant symbol c in τ. On the other hand, we call $\mathcal{A}$ a *σ-expansion* of $\mathcal{A}_{|\tau}$.

To indicate that two σ-structures $\mathcal{A}$ and $\mathcal{B}$ are *isomorphic*, we write $\mathcal{A} \cong \mathcal{B}$.

In the following, suppose that σ is a relational signature. We say that $\mathcal{B}$ is a *substructure* of $\mathcal{A}$ if $B \subseteq A$ and $R^{\mathcal{B}} \subseteq R^{\mathcal{A}}$ for each relation symbol R from σ. The structure $\mathcal{B}$ is an *induced substructure* of $\mathcal{A}$ if $\mathcal{B}$ is a substructure of $\mathcal{A}$ and $R^{\mathcal{B}} = R^{\mathcal{A}} \cap B^r$ for each relation symbol R of arity $r \geq 1$ from σ. We then say that $\mathcal{B}$ is the substructure of $\mathcal{A}$ *induced* by the set B.

For every set B such that $A \cap B \neq \emptyset$, we write $\mathcal{A}[B]$ to denote the substructure of $\mathcal{A}$ induced by $A \cap B$. Furthermore, if $A \setminus B \neq \emptyset$ then $\mathcal{A} \setminus B$ is the induced substructure $\mathcal{A}[A \setminus B]$ of $\mathcal{A}$ obtained by deleting all elements from B.

Two σ-structures are *disjoint*, if their universes are disjoint. Let $s \geq 1$, and let $\mathcal{A}_1, \ldots, \mathcal{A}_s$ be (not necessarily disjoint) σ-structures. The *union* $\mathcal{A}_1 \cup \cdots \cup \mathcal{A}_s$ of $\mathcal{A}_1, \ldots, \mathcal{A}_s$ is the σ-structure $\mathcal{C}$ with universe $A_1 \cup \cdots \cup A_s$ where, for each relation symbol R from σ, the relation $R^{\mathcal{C}}$ is the union of the relations $R^{\mathcal{A}_1}, \ldots, R^{\mathcal{A}_s}$.

A σ-structure $\mathcal{D}$ is called a *disjoint union of* $\mathcal{A}_1, \ldots, \mathcal{A}_s$ if it is the union of pairwise disjoint σ-structures $\mathcal{A}'_1, \ldots, \mathcal{A}'_s$, that is, of σ-structures whose universes are pairwise disjoint, such that $\mathcal{A}'_i \cong \mathcal{A}_i$ for each $i \in [1, s]$.

2.4 Logics

In this section, we define the logics used in this thesis. The notation introduced is based on [EF99]. We commence with the standard notation for propositional logic, which we need for a definition of so-called reduction sequences in Chapter 5. The main part of this section will provide the syntax and semantics of the logics in the focus of this thesis, that is, first-order logic and its extensions by unary counting quantifiers. For each such logic, we will also define an extension by tuple-counting quantifiers.

2.4.1 Propositional Logic

By PS we denote a countable set of *propositional symbols*. PL is the set of *propositional formulae*, that is, the smallest set of formulae that is closed under *atomic propositional formulae* (A) and *Boolean connectives* (B) as described below:

(A) $\mathsf{PS} \subseteq \mathsf{PL}$ and $\mathbf{0}, \mathbf{1} \in \mathsf{PL}$.

(B) If $\varphi, \psi \in \mathsf{PL}$, then also $\neg\varphi \in \mathsf{PL}$ and $(\varphi \vee \psi) \in \mathsf{PL}$.

We omit parentheses if this does not lead to ambiguity, and we treat the Boolean connectives $\varphi \wedge \psi$, $\varphi \rightarrow \psi$, and $\varphi \leftrightarrow \psi$, as abbreviations for the formulae $\neg(\neg\varphi \vee \neg\psi)$, $\neg\varphi \vee \psi$, and $(\varphi \rightarrow \psi) \wedge (\psi \rightarrow \varphi)$, respectively.

A propositional formula φ is represented by a word $\mathrm{rep}(\varphi)$ over the alphabet $\mathsf{PS} \cup \{\neg, \vee, (,), \mathbf{0}, \mathbf{1}\}$. The *size* $||\varphi||$ of φ is the length of $\mathrm{rep}(\varphi)$.

A *propositional interpretation* is a function $\mu \colon \mathsf{PS} \rightarrow \{0, 1\}$. For any formula $\varphi \in \mathsf{PL}$ we write $\mu \models \varphi$ to express that μ is a *model* of φ (and we write $\mu \not\models \varphi$ if this is not the case). The model relation is defined recursively as follows:

(A) $\mu \models \mathbf{1}$ and $\mu \not\models \mathbf{0}$, and for each $X \in \mathsf{PS}$,

$$\mu \models X \quad \text{iff} \quad \mu(X) = 1.$$

(B) For $\varphi, \psi \in \mathsf{PL}$,

$$\mu \models \neg\varphi \quad \text{iff} \quad \mu \not\models \varphi$$

and

$$\mu \models \varphi \vee \psi \quad \text{iff} \quad \mu \models \varphi \ \text{ or } \ \mu \models \psi.$$

2.4.2 First-Order Logic and Unary Counting Quantifiers

By Var we denote a countable set of *variable symbols*, which we will also call *variables* for short. Variables will be the only terms allowed in the formulae introduced in the sequel. In particular, *no constant or function symbols are used.* Every logic L considered in this thesis contains all *atomic formulae* (A) and is closed under *Boolean connectives* (B). More precisely, the set of formulae in any logic L adheres to the following rules:

(A) If $x, y \in \mathsf{Var}$, then $x{=}y \in \mathsf{L}$, and
if $R \in \mathsf{Rel}$ is of arity $r \geq 1$ and $x_1, \ldots, x_r \in \mathsf{Var}$, then $R(x_1, \ldots, x_r) \in \mathsf{L}$.

(B) If $\varphi, \psi \in \mathsf{L}$, then also the formulae $\neg\varphi$ and $\varphi \vee \psi$ belong to L.

We treat the Boolean connectives $\varphi \wedge \psi$, $\varphi \to \psi$, and $\varphi \leftrightarrow \psi$ as abbreviations for the formulae $\neg(\neg\varphi \vee \neg\psi)$, $\neg(\varphi \vee \psi)$, and $(\varphi \to \psi) \wedge (\psi \to \varphi)$, respectively.

Whenever we speak about a logic L in this thesis, we will mean one of the logics defined below. For a relational signature σ, we denote by $\mathsf{L}[\sigma]$ the subset of the logic L that contains all formulae from L that only make use of the relation symbols occurring in σ.

The formulae of all logics defined in the following are built from atomic formulae and Boolean connectives, as described above, and are distinguished by the allowed quantifiers.

Unary Counting Quantifiers

As we only consider finite structures, we understand a *unary counting quantifier* Q (for short: *quantifier*) as a subset of the natural numbers (cf., e.g., [LN00, Nur00]). Broadly speaking, the numbers in this set represent the cardinalities of the witness sets accepted by the quantifier. More formal semantics for the logics using such quantifiers are given further down below. We will also allow derived quantifiers $(\mathsf{Q}{+}k)$ that increment the numbers in the set Q by a constant $k \in \mathbb{N}$, that is,

$$(\mathsf{Q}{+}k) \;:=\; \{n{+}k \,:\, n \in \mathsf{Q}\}.$$

Clearly, $(\mathsf{Q}{+}0) = \mathsf{Q}$.

Example 2.4.1. As we only consider finite structures, the existential quantifier $\exists$ can be defined by the set of all natural numbers ≥ 1. For each $k \geq 0$, the *threshold-counting quantifier* $(\exists{+}k)$ is given by the set of all natural numbers $> k$.

Other examples for unary counting quantifiers are the set of all prime numbers, and the set of all natural numbers representing (in a suitable encoding) Turing machines (cf., e.g., [EF99]) that halt on the empty input.

By C_{all} we denote the *set of all unary counting quantifiers*, that is, the set $\mathcal{P}(\mathbb{N})$ of all subsets of the natural numbers. In the following, we define a series of logics, starting with first-order logic and closing with the extension of first-order logic by arbitrary unary counting quantifiers from C_{all}. In another direction, we will extend each of these logics to a logic whose quantifiers can also count tuples of elements instead of only single elements. When we talk about some abstract logic in the sequel, we will always mean one of the logics defined below.

After defining the syntax of the considered logics, we will define some crucial parameters of logic formulae as, e.g., the quantifier rank, and conclude the section by providing semantics for these logics.

Plain First-Order Logic

Plain first-order logic (for short: FO) is the smallest set of formulae that is closed under the rules (A), (B), and the following rule for *existential quantification*:

(∃) If $\varphi \in \mathsf{FO}$ and $x \in \mathsf{Var}$, then $\exists x\, \varphi \in \mathsf{FO}$.

We treat *universal quantification* $\forall x\, \varphi$ as an abbreviation for the formula $\neg\exists x\, \neg\varphi$.

First-Order Logic with Threshold-Counting

First-order logic with threshold-counting (for short: $\mathsf{FO{+}unT}$) additionally allows *threshold-counting.* That is, $\mathsf{FO{+}unT}$ is the smallest set of formulae that is closed under the rules (A), (B), and the following generalisation to the rule (∃):

(T) If $\varphi \in \mathsf{FO{+}unT}$, $x \in \mathsf{Var}$, and $k \geq 0$, then $(\exists{+}k)x\, \varphi \in \mathsf{FO{+}unT}$.

Clearly, $\mathsf{FO} \subset \mathsf{FO{+}unT}$.

First-Order Logic with Modulo-Counting

A *modulo-counting quantifier with period* $p \geq 2$ is a unary counting quantifier that is defined by the subset

$$\mathsf{D}_p \;\coloneqq\; \{n \in \mathbb{N} \,:\, n \text{ is divisible by } p\}$$

of the natural numbers (cf., e.g., [Nur00]). By D_{all}, we denote the *set of all modulo-counting quantifiers* for arbitrary periods $p \geq 2$.

For every set $D \subseteq D_{\text{all}}$, *first-order logic with modulo-counting quantifiers from* D (for short: $\mathsf{FO{+}unM}(D)$) is the smallest set of formulae that is closed under (A), (B), (T), and the following rule:

(D) If $\varphi \in \mathsf{FO{+}unM}(D)$, $x \in \mathsf{Var}$, $\mathsf{D}_p \in D$, and $r \in [0, p)$, then $(\mathsf{D}_p{+}r)x\, \varphi \in \mathsf{FO{+}unM}(D)$.

In the following, we also abbreviate $\mathsf{FO{+}unM}(D_{\text{all}})$ by $\mathsf{FO{+}unM}$.

First-Order Logic with Arbitrary Unary Counting Quantifiers

For an arbitrary set $C \subseteq C_{\text{all}}$ of unary counting quantifiers, *first-order logic with counting quantifiers from* C (for short: $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)$) is the smallest set of formulae that is closed under (A), (B), (T), and the following rule:

(C) If $\varphi \in \mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)$, $x \in \mathsf{Var}$, $\mathsf{Q} \in C$, and $k \geq 0$, then $(\mathsf{Q}{+}k)x\,\varphi \in \mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)$.

For short, we also write $\mathsf{FO}{+}\mathrm{un}\mathsf{C}$ for $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C_{\text{all}})$.

Logics with Tuple-Counting Quantifiers

For any logic L of the aforementioned ones, we denote by L_{tpl} the logic where each quantifier allowed in L is allowed to count over finite tuples. That is, L_{tpl} is the smallest set of formulae that adheres to the rules describing the logic L as defined above, and the following rule for *tuple-counting quantifiers* (cf., [Str94]):

(tpl) If $\mathsf{Q}x\,\varphi \in \mathsf{L}_{\text{tpl}}$ for some $\mathsf{Q} \subseteq \mathbb{N}$ and $x \in \mathsf{Var}$, then also $\mathsf{Q}(x_1, \ldots, x_m)\,\varphi \in \mathsf{L}_{\text{tpl}}$ for any tuple $(x_1, \ldots, x_m)$ of $m \geq 1$ pairwise distinct variables.

Note that $\mathsf{L} \subseteq \mathsf{L}_{\text{tpl}}$ and that $(\mathsf{L}_{\text{tpl}})_{\text{tpl}} = \mathsf{L}_{\text{tpl}}$.

Alternative Notation for Threshold- and Modulo-Counting Quantifiers

For a better readability, we will also use the following abbreviations in the sequel. Let φ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}_{\text{tpl}}$ and let $\overline{x}$ be a non-empty tuple of pairwise distinct variables. Then,

$$
\begin{array}{rcll}
\exists^{>k}\overline{x}\,\varphi & := & (\exists{+}k)\overline{x}\,\varphi & \text{for each } k \geq 0, \\
\exists^{\geq k}\overline{x}\,\varphi & := & (\exists{+}(k{-}1))\overline{x}\,\varphi & \text{for each } k \geq 1, \\
\exists^{=k}\overline{x}\,\varphi & := & \exists^{\geq k}\overline{x}\,\varphi \;\wedge\; \neg\exists^{>k}\overline{x}\,\varphi & \text{for all } k \geq 1, \\
\exists^{=0}\overline{x}\,\varphi & := & \neg\exists\overline{x}\,\varphi, & \text{and} \\
\exists^{\equiv r \bmod p}\overline{x}\,\varphi & := & (\mathsf{D}_p{+}r)\overline{x}\,\varphi & \text{for all } p \geq 2 \text{ and } r \in [0, p).
\end{array}
$$

Properties of Formulae

Let L be one of the logics defined above and consider an L-formula φ.

The *quantifier rank* $\mathrm{qr}(\varphi)$ and the *set of free variables* $\mathrm{free}(\varphi)$ are defined inductively over the shape of φ as follows: If φ is an atomic formula, then

$\mathrm{qr}(\varphi) \coloneqq 0$ and $\mathrm{free}(\varphi)$ is the set of all variables from Var that appear in φ. If φ is of the shape $\neg\varphi'$, then $\mathrm{qr}(\varphi) \coloneqq \mathrm{qr}(\varphi')$ and $\mathrm{free}(\varphi) \coloneqq \mathrm{free}(\varphi')$; and if φ is of the shape $\varphi' \vee \varphi''$, then $\mathrm{qr}(\varphi)$ is the maximum of $\mathrm{qr}(\varphi')$ and $\mathrm{qr}(\varphi'')$, and $\mathrm{free}(\varphi)$ is the union of $\mathrm{free}(\varphi')$ and $\mathrm{free}(\varphi'')$. Finally, suppose that φ is of the shape $\mathsf{Q}(x_1, \dots, x_m)\, \varphi'$ for a tuple $(x_1, \dots, x_m)$ of $m \geq 1$ pairwise distinct variables. Then, $\mathrm{qr}(\varphi) \coloneqq m + \mathrm{qr}(\varphi')$ and $\mathrm{free}(\varphi) \coloneqq \mathrm{free}(\varphi') \setminus \{x_1, \dots, x_m\}$. In particular, φ is called *quantifier-free* if $\mathrm{qr}(\varphi) = 0$.

The *dimension* of φ is 1 if φ is quantifier-free, and otherwise it is the maximum length of all variable tuples $\overline{x}$ for which φ contains a subformula of the shape $\mathsf{Q}\overline{x}\,\psi$ for some unary counting quantifier Q.

For formulae φ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ (and thus, in particular, formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}_{\mathrm{tpl}}$), we define two additional parameters: The *threshold* of φ is the smallest $K \geq 0$ such that every subformula of the shape $(\exists{+}k)\overline{x}\,\psi$ has $k \leq K$, and the *maximum period* of φ is the smallest $P \geq 0$ such that every subformula of the shape $(\mathsf{D}_p{+}r)\overline{x}\,\psi$ for some $p \geq 2$ and $r \in [0, p)$ has $p \leq P$.

Semantics

In the following, we fix a relational signature σ. A *σ-interpretation* is a tuple $(\mathcal{A}, \beta)$, consisting of a σ-structure $\mathcal{A}$ and a function $\beta\colon \mathsf{Var} \to A$. The *universe of* $(\mathcal{A}, \beta)$ is the universe A of $\mathcal{A}$.

For a logic L as defined above and a formula $\varphi \in \mathsf{L}[\sigma]$, we write $(\mathcal{A}, \beta) \models \varphi$ to express that $(\mathcal{A}, \beta)$ is a *model* of φ (and we write $(\mathcal{A}, \beta) \not\models \varphi$ if this is not the case). The model relation is defined recursively as follows:

(A) For variables $x, y \in \mathsf{Var}$,

$$(\mathcal{A}, \beta) \ \models \ x{=}y \quad \text{iff} \quad \beta(x) \ = \ \beta(y).$$

For each relation symbol R from σ with arity $r \geq 1$ and all $x_1, \dots, x_r \in \mathsf{Var}$,

$$(\mathcal{A}, \beta) \ \models \ R(x_1, \dots, x_r) \quad \text{iff} \quad (\beta(x_1), \dots, \beta(x_r)) \ \in \ R^{\mathcal{A}}.$$

(B) For formulae φ, ψ from $\mathsf{L}[\sigma]$,

$$(\mathcal{A}, \beta) \ \models \ \neg\varphi \quad \text{iff} \quad (\mathcal{A}, \beta) \ \not\models \ \varphi$$

and

$$(\mathcal{A}, \beta) \ \models \ \varphi \vee \psi \quad \text{iff} \quad (\mathcal{A}, \beta) \ \models \ \varphi \ \text{ or } \ (\mathcal{A}, \beta) \ \models \ \psi.$$

(C) For any formula $\mathsf{Q}(x_1, \ldots, x_m)\,\varphi$ that belongs to $\mathsf{L}[\sigma]$, where $\mathsf{Q} \subseteq \mathbb{N}$ and where $(x_1, \ldots, x_m)$ is a tuple of $m \geq 1$ pairwise distinct variables,

$$\begin{aligned} & (\mathcal{A}, \beta) \;\models\; \mathsf{Q}(x_1, \ldots, x_m)\,\varphi \\ \text{iff} \quad & \left|\left\{(a_1, \ldots, a_m) \in A^m \colon \left(\mathcal{A}, \beta\tfrac{a_1,\ldots,a_m}{x_1,\ldots,x_m}\right) \models \varphi\right\}\right| \;\in\; \mathsf{Q}. \end{aligned}$$

In the latter equivalence, $\beta\frac{a_1,\ldots,a_m}{x_1,\ldots,x_m}$ denotes the function $\beta' \colon \mathsf{Var} \to A$ with $\beta'(x_i) \coloneqq a_i$ for all $i \in [1, m]$ and $\beta'(z) \coloneqq \beta(z)$ for all $z \in \mathsf{Var} \setminus \{x_1, \ldots, x_m\}$.

For a tuple $\overline{x} = (x_1, \ldots, x_n)$ of pairwise distinct variables and a formula φ from L, we write $\varphi(\overline{x})$ to express that $\text{free}(\varphi) \subseteq \{x_1, \ldots, x_n\}$. Note that this also induces an order on the free variables of φ.

For a σ-structure $\mathcal{A}$ and a tuple $\overline{a} = (a_1, \ldots, a_n) \in A^n$, the tuple $(\mathcal{A}, \overline{a})$ denotes the interpretation $(\mathcal{A}, \beta)$ for $\varphi(\overline{x})$ where $\beta \colon \mathsf{Var} \to A$ is defined such that $\beta(x_i) = a_i$ for all $i \in [1, n]$ and such that $\beta(y) = a$ for all $y \in \mathsf{Var} \setminus \{x_1, \ldots, x_n\}$ and an arbitrary but fixed element $a \in A$. In particular, we write $(\mathcal{A}, \overline{a}) \models \varphi$ (for short: $\mathcal{A} \models \varphi[\overline{a}]$) to express that $(\mathcal{A}, \beta)$ is a model of $\varphi(\overline{x})$.

For a class $\mathfrak{C}$ of σ-structures, two formulae $\varphi(\overline{x})$ and $\psi(\overline{x})$ from $\mathsf{L}[\sigma]$ are $\mathfrak{C}$-*equivalent*, if

$$\mathcal{A} \;\models\; \varphi[\overline{a}] \quad \text{iff} \quad \mathcal{A} \;\models\; \psi[\overline{a}]$$

for each structure $\mathcal{A} \in \mathfrak{C}$ and every tuple $\overline{a} \in A^n$. The formulae $\varphi(\overline{x})$ and $\psi(\overline{x})$ are called *equivalent* if they are $\mathfrak{C}$-equivalent for the class $\mathfrak{C}$ of all σ-structures.

2.5 Ultimately Periodic Quantifiers

In this section, we introduce so-called *ultimately periodic* unary counting quantifiers (cf. [Mat94]). Ultimately periodic quantifiers will turn out to be the largest class of unary counting quantifiers for which most of the results of this thesis are applicable. In contrast to unary counting quantifiers in general, ultimately periodic quantifiers can be represented by suitable finite words and thus allow us to define a finite encoding of formulae that only use ultimately periodic quantifiers.

Intuitively, ultimately periodic quantifiers are unary counting quantifiers that can be obtained from threshold-counting and modulo-counting quantifiers by a finite number of applications of the set-theoretic operations complement and union. However, another characterisation will turn out to be more useful for our purposes:

Definition 2.5.1. A unary counting quantifier $\mathsf{Q} \subseteq \mathbb{N}$ is *ultimately periodic* if there exist numbers $p, n_0 \in \mathbb{N}$ with $p \geq 1$, such that

$$\text{for all } n \geq n_0 \text{ we have} \quad n \in \mathsf{Q} \quad \text{iff} \quad n + p \in \mathsf{Q}\,.$$

The *period* of Q is the minimal $p \geq 1$ for which the latter property is true for some n_0. The number n_0 is called an *offset* of Q.

We denote the *set of all ultimately periodic unary counting quantifiers* by U_{all}.

Example 2.5.2. The existential quantifier and all quantifiers $(\mathsf{D}_p{+}r)$ with $p \geq 2$ and $r \in [0, p)$ are ultimately periodic with period 1 and offset 1, and with period p and offset r, respectively. More generally, if $\mathsf{Q} \subseteq \mathbb{N}$ is ultimately periodic with period $p \geq 1$ and offset $n_0 \geq 0$, then, for each $k \geq 0$, the quantifier $(\mathsf{Q}{+}k)$ is ultimately periodic with period p and offset $n_0 + k$.

As a counterexample, the sets of all square numbers or all prime numbers are not ultimately periodic.

We call a logic L as defined in Section 2.4.2 *ultimately periodic* if all quantifiers permitted in the logic are ultimately periodic.

Example 2.5.3. All the logics FO, $\mathsf{FO}{+}\text{un}\mathsf{T}$, $\mathsf{FO}{+}\text{un}\mathsf{M}(D)$ for all $D \subseteq D_{\text{all}}$, and $\mathsf{FO}{+}\text{un}\mathsf{C}(U)$ for all $U \subseteq U_{\text{all}}$, as well as their tuple-counting extensions, are ultimately periodic.

Until now we have described unary counting quantifiers by sets of natural numbers. In the following, we provide an alternative description, which is useful for encoding ultimately periodic quantifiers, as well as for applying word combinatorial reasoning to them (see Chapter 8).

Definition 2.5.4. The *characteristic sequence of a quantifier* $\mathsf{Q} \subseteq \mathbb{N}$ is the ω-word $\chi_{\mathsf{Q}} \coloneqq w_0 w_1 w_2 \ldots$ over the alphabet $\{0, 1\}$ where, for each $i \in \mathbb{N}$,

$$w_i = 1 \quad \text{iff} \quad i \in \mathsf{Q}.$$

A finite word $w \in \{0,1\}^*$ is *primitive* (cf., e.g., [Lot84]) if for every word $u \in \{0,1\}^*$, $w \in u^*$ implies $w = u$. Any finite non-empty word $\pi \in \{0,1\}^*$ can be written as w^n for some primitive word $w \in \{0,1\}^*$ and some $n \geq 1$. Note that this primitive word w is uniquely determined by π and thus called the *primitive root* of π.

The following fact defines an ultimately periodic quantifier in terms of its characteristic sequence.

Fact 2.5.5. For every $\mathsf{Q} \subseteq \mathbb{N}$, the following holds:

- If Q is ultimately periodic with period $p \geq 1$ and offset $n_0 \geq 0$, then there is a word $\alpha \in \{0,1\}^*$ of length n_0 and a primitive word $\pi \in \{0,1\}^+$ of length p such that $\chi_{\mathsf{Q}} = \alpha\pi^\omega$.
- If $\chi_{\mathsf{Q}} = \alpha\pi^\omega$ for finite words $\alpha \in \{0,1\}^*$ and $\pi \in \{0,1\}^+$, then Q is ultimately periodic, its period is the length of the primitive root of π, and $|\alpha|$ is an offset.

Thus, we can represent an ultimately periodic quantifier Q by the finite word $\mathrm{rep}(\mathsf{Q}) \coloneqq \alpha\#\pi$ over the alphabet $\{0,1,\#\}$, where $\chi_{\mathsf{Q}} = \alpha\pi^\omega$. To make this definition unambiguous, we demand that $p \coloneqq |\pi|$ is the period of Q, and $n_0 \coloneqq |\alpha|$ is the *smallest* offset of Q. The *size* $||\mathsf{Q}||$ of Q is the length of $\mathrm{rep}(\mathsf{Q})$.

In particular, $||\mathsf{Q}|| = n_0 + p + 1 \geq 2$ and $||(\mathsf{Q}{+}k)|| = ||\mathsf{Q}|| + k$ for all $k \geq 0$.

Example 2.5.6. The existential quantifier is represented by the word $\mathrm{rep}(\exists) = 0\#1$. On the other hand, for every period $p \geq 2$ and each remainder $r \in [0,p)$, the modulo-counting quantifier with period p and remainder r is represented by the word $\mathrm{rep}((\mathsf{D}_p{+}r)) = 0^r\#10^{p-1}$.

Using this representation, any formula φ from any ultimately periodic logic can be represented by a word $\mathrm{rep}(\varphi)$ over the alphabet

$$\mathsf{Var} \;\cup\; \mathsf{Rel} \;\cup\; \{,\} \;\cup\; \{=,\neg,\vee,(,),0,1,\#\},$$

where each quantifier $\mathsf{Q} \in U_{\mathrm{all}}$ is represented by the word $\mathrm{rep}(\mathsf{Q})$. The *size* $||\varphi||$ of φ is the length of $\mathrm{rep}(\varphi)$.

2.6 Transductions

The following introduction to transductions[1] is based on [EF99, Gru16, Gro17]. For the following, we let L denote one of the logics defined in the previous sections. In this thesis, we will only consider first-order transductions.

Broadly spoken, for relational signatures σ and τ, a transduction Θ from σ to τ is a tuple of formulae from $\mathsf{FO}[\sigma]$. The satisfying assignments for the free variables of these formulae in respect to a σ-structure $\mathcal{A}$ define the universe and the relations of an associated τ-structure $\Theta[\mathcal{A}]$. On the other hand, given a formula φ from $\mathsf{L}[\tau]$, the transduction can be used to transform φ into a so-called

[1] also called *logical (or: syntactical) interpretations* (cf., e.g., [EF99])

Θ-reduct $\varphi^{-\Theta}$ of φ, which is a formula of $\mathsf{L}_{\mathrm{tpl}}[\sigma]$ that, in a σ-structure $\mathcal{A}$, has the same meaning as φ in the τ-structure $\Theta[\mathcal{A}]$.

The so-called *transduction lemma*, stated further at the end of Section 2.6, describes the crucial relationship between the structure $\Theta[\mathcal{A}]$ and the Θ-reduct formally.

For the following, we fix two relational signatures σ and τ. In particular, we suppose that $\tau = (R_1, \ldots, R_\ell)$ for an $\ell \geq 0$ and a relation symbol R_i of arity $r_i \geq 1$ for each $i \in [1, \ell]$.

Definition 2.6.1. Let $t \geq 1$, let

- $\theta(x_1, \ldots, x_t)$ be an $\mathsf{FO}[\sigma]$-formula, and let
- $\theta_{R_i}(\overline{y}_1, \ldots, \overline{y}_{r_i})$, for each $i \in [1, \ell]$, be a formula from $\mathsf{FO}[\sigma]$ with the variable tuples $\overline{y}_j \coloneqq (y_{j,1}, \ldots, y_{j,t})$ for all $j \in [1, r_i]$.

The tuple $\Theta = (\theta, \theta_{R_1}, \ldots, \theta_{R_\ell})$ is called a *transduction from σ to τ with arity t.*

The *quantifier rank* $\mathrm{qr}(\Theta)$ and the *size* $||\Theta||$ of Θ are the *maximum* of the quantifier rank and the size of the formulae $\theta, \theta_{R_1}, \ldots, \theta_{R_\ell}$, respectively.

Example 2.8.3 further down below provides an example of a transduction that turns structures over σ into their so-called Gaifman-graph.

The following definition describes the application of a transduction from σ to τ to a σ-structure. To avoid ambiguity, we introduce a notation to explicitly denote tuples of tuples. Recall that, for tuples $\overline{b}_1, \ldots, \overline{b}_n$, the expression $(\overline{b}_1, \ldots, \overline{b}_n)$ usually denotes the concatenation of these tuples, i.e., a tuple of length $|\overline{b}_1| + \cdots + |\overline{b}_n|$. To denote the tuple of length n whose elements are the tuples $\overline{b}_1, \ldots, \overline{b}_n$, we will use the expression $(\overline{b}_1; \ldots; \overline{b}_n)$ from now on.

Definition 2.6.2. Let $\Theta = (\theta, \theta_{R_1}, \ldots, \theta_{R_\ell})$ be a transduction from σ to τ with arity $t \geq 1$. Let $\mathcal{A}$ be a σ-structure such that the set

$$B \quad \coloneqq \quad \{\overline{b} \in A^t \,:\, \mathcal{A} \models \theta[\overline{b}]\}.$$

is not empty. Then, the *application* $\Theta[\mathcal{A}]$ *of* Θ *to* $\mathcal{A}$ is defined, and given by the τ-structure

$$\mathcal{B} \quad \coloneqq \quad (B, R_1^{\mathcal{B}}, \ldots, R_\ell^{\mathcal{B}})$$

where, for each $i \in [1, \ell]$,

$$R_i^{\mathcal{B}} \quad \coloneqq \quad \{(\overline{b}_1; \ldots; \overline{b}_{r_i}) \in B^{r_i} \,:\, \mathcal{A} \models \theta_{R_i}[\overline{b}_1, \ldots, \overline{b}_{r_i}]\}.$$

For a transduction Θ from σ to τ, a Θ-reduct of an $\mathsf{L}[\tau]$-sentence φ is an $\mathsf{L}'[\sigma]$-sentence over a logic L' that is satisfied by a σ-structure $\mathcal{A}$ whenever the τ-structure $\Theta[\mathcal{A}]$ satisfies φ. The following definition makes this precise and also covers formulae with free variables.

Definition 2.6.3. Let Θ be a transduction from σ to τ with arity $t \geq 1$, and let $\varphi(\overline{x})$ be a formula from $\mathsf{L}[\tau]$ with free variables from a tuple $\overline{x} = (x_1, \dots, x_n)$ of length $n \geq 0$. A Θ-*reduct of* $\varphi(\overline{x})$ is a formula $\psi(\overline{x}_1, \dots, \overline{x}_n)$ from $\mathsf{L}'[\sigma]$, for some logic L', with free variables from the tuples $\overline{x}_i \coloneqq (x_{i,1}, \dots, x_{i,t})$ for all $i \in [1, n]$, for which the following holds: If $\mathcal{A}$ is a σ-structure for which $\Theta[\mathcal{A}]$ is defined and $\overline{b}_1, \dots, \overline{b}_n$ are elements from the universe of $\Theta[\mathcal{A}]$, then

$$\begin{array}{rrcl} & \Theta[\mathcal{A}] & \models & \varphi[\overline{b}_1; \dots; \overline{b}_n] \\ \text{iff} & \mathcal{A} & \models & \psi[\overline{b}_1, \dots, \overline{b}_n]. \end{array}$$

Note that Θ-reducts are not defined uniquely, but just as formulae of some logic with the semantic property described above. This will be useful later in Chapter 5, where we transform Θ-reducts using tuple-counting quantifiers into equivalent formulae without tuple-counting quantifiers, which we also want to treat as Θ-reducts.

The following transduction lemma shows that for each transduction Θ from σ to τ and every formula $\varphi \in \mathsf{L}[\tau]$, a canonically defined Θ-reduct $\varphi^{-\Theta}$ of φ exists in $\mathsf{L}_{\mathrm{tpl}}[\sigma]$. Here, tuple-counting quantifiers are only necessary if Θ has arity ≥ 2. I.e., if Θ has arity 1, then $\varphi^{-\Theta}$ belongs to $\mathsf{L}[\sigma]$.

The lemma also provides upper bounds on the quantifier rank, number of free variables, and dimension of the Θ-reduct. For ultimately periodic L, also upper bounds on the size and the time required for the construction of the Θ-reduct are given. Furthermore, for the special case of input formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$, also the threshold and the maximum period of Θ-reducts are examined.

Lemma 2.6.4. *Let σ and τ be relational signatures, and let Θ be a transduction from σ to τ with arity $t \geq 1$. Let L be a logic. For every formula φ from $\mathsf{L}[\tau]$, there is a Θ-reduct $\varphi^{-\Theta}$ in $\mathsf{L}_{\mathrm{tpl}}[\sigma]$.*

Suppose that $q, n \geq 0$ and $m \geq 1$ are the quantifier rank, the number of free variables, and the dimension of φ, respectively, and that $q_\Theta \geq 0$ is the quantifier rank of Θ. The formula $\varphi^{-\Theta}$ has quantifier rank $\leq t \cdot q + q_\Theta$, $t \cdot n$ free variables, and dimension $\leq t \cdot m$.

Moreover, if L *is ultimately periodic, there is an algorithm which, on input of* Θ *and* φ*, computes* $\varphi^{-\Theta}$ *in time*

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + ||\Theta|| \cdot \mathcal{O}(||\varphi||)$$

and of size $||\Theta|| \cdot \mathcal{O}(||\varphi||)$*.*

Finally, if $\varphi \in \mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\tau]$ *then* $\varphi^{-\Theta} \in \mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ *has the same threshold and maximum period as* φ*.*

Proof. Let σ and τ be relational signatures and suppose that $\tau = (R_1, \dots, R_\ell)$ for an $\ell \geq 0$ and a relation symbol R_i of arity $r_i \geq 1$ for each $i \in [1, \ell]$. Let $\Theta = (\theta, \theta_{R_1}, \dots, \theta_{R_\ell})$ be a transduction from τ to σ with arity $t \geq 1$ and quantifier rank $q_\Theta \geq 0$. Furthermore, let L be a logic and $\varphi(\overline{x})$ a formula from $\mathsf{L}[\tau]$ with a tuple $\overline{x} = (x_1, \dots, x_n)$ of $n \geq 0$ free variables, quantifier rank $q \geq 0$, and dimension $m \geq 1$.

Let $v_0, v_1, v_2, \dots$ be a sequence of variables from Var. Without loss of generality we suppose that $\varphi(\overline{x})$ only uses variables from the sequence $v_0, v_t, v_{2t}, \dots$. That is, for any variable x in φ, there is an $i \geq 0$ such that $x = v_{i \cdot t}$. This way, the variable $x_j \coloneqq v_{i \cdot t + j - 1}$, for each $j \in [1, t]$, does not occur in φ. In particular, we let $\overline{x}_i \coloneqq (x_{i,1}, \dots, x_{i,t})$ for each $i \in [1, n]$.

Recall that $||\Theta||$ is the maximum of the size of the formulae $\theta, \theta_{R_1}, \dots, \theta_{R_\ell}$. Thus, to read the transduction Θ takes time in $||\Theta|| \cdot \mathcal{O}(||\tau||)$. Afterwards, the construction of $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ from $\varphi(x_1, \dots, x_n)$ proceeds by an induction over the shape of $\varphi(x_1, \dots, x_n)$, where we show the following inductive invariant to hold:

Claim 1.

(i) $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ *is a* Θ*-reduct of* $\varphi(x_1, \dots, x_n)$ *that belongs to* $\mathsf{L}_{\mathrm{tpl}}[\sigma]$

(ii) $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ *has dimension* $\leq t \cdot m$*.*

(iii) $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ *has quantifier rank* $\leq t \cdot q + q_\Theta$*.*

(iv) If $\varphi \in \mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\tau]$ *then* $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n) \in \mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ *has the same threshold and maximum period as* φ*.*

(v) For an ultimately periodic logic L*, there is an algorithm that takes at most*

$$c \cdot ||\Theta|| \cdot ||\varphi||$$

time steps to compute $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$*, for a suitable number* $c \in \mathbb{N}_{\geq 1}$*.*

We start by a description of the construction of $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ and by showing the validity of the Statements (i) to (iv). Afterwards, we conclude with an analysis of the running time of the algorithm, which, for ultimately periodic L, is implied by the construction.

If $\varphi(x_1, \dots, x_n)$ is of the shape $x_{i_1}{=}x_{i_2}$ for indices $\{i_1, i_2\} = [1, n]$, let

$$\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n) \;\coloneqq\; \bigwedge_{i=1}^{n} \theta(\overline{x}_i) \;\wedge\; \bigwedge_{j=1}^{t} x_{i_1,j}{=}x_{i_2,j}.$$

Since Θ only uses $\mathsf{FO}[\sigma]$-formulae, $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ belongs to $\mathsf{FO}[\sigma]$. Thus, in particular, it has dimension 1, threshold 0, maximum period 0, and quantifier rank $\leq q_\Theta$. By definition of $\Theta[\mathcal{A}]$ for σ-structures $\mathcal{A}$ it is straightforward to verify that $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ indeed is a Θ-reduct of $\varphi(x_1, \dots, x_n)$. Hence, Statements (i) to (iv) of Claim 1 are satisfied.

If φ is of the shape $R_i(x_{j_1}, \dots, x_{j_{r_i}})$ for $i \in [1, \ell]$ and indices $\{j_1, \dots, j_{r_i}\} = [1, n]$, let

$$\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n) \;\coloneqq\; \bigwedge_{i=1}^{n} \theta(\overline{x}_i) \;\wedge\; \theta_{R_i}(\overline{x}_{j_1}, \dots, \overline{x}_{j_{r_i}}).$$

Clearly, $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ belongs to $\mathsf{FO}[\sigma]$. It follows directly from the definition of $\Theta[\mathcal{A}]$ for σ-structures $\mathcal{A}$, that the formula $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ is a Θ-reduct for $\varphi(x_1, \dots, x_n)$ and thus, Statement (i) of Claim 1 holds. Furthermore, by construction, $\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n)$ has dimension 1, threshold 0, maximum period 0, and quantifier rank $\leq q_\Theta$. Therefore, also Statements (ii) to (iv) hold.

For a Boolean combination $\varphi(\overline{x})$, the translation distributes. That is, we let $(\neg\varphi')^{-\Theta} \coloneqq \neg(\varphi')^{-\Theta}$ and $(\varphi' \vee \varphi'')^{-\Theta} \coloneqq (\varphi')^{-\Theta} \vee (\varphi'')^{-\Theta}$. Clearly, Statements (i) to (iv) of Claim 1 are satisfied in both cases.

Suppose that $\varphi(\overline{x}) = (\mathsf{Q}{+}k)\overline{y}\,\psi(\overline{x}, \overline{y})$ for some quantifier $\mathsf{Q} \subseteq \mathbb{N}$ permitted in L, a number $k \geq 0$, and a tuple $\overline{y} = (y_1, \dots, y_{m'})$ of $m' \in [1, m]$ pairwise distinct variables. By Statement (i) of Claim 1 we know that $\mathsf{L}_{\mathrm{tpl}}[\sigma]$ contains a Θ-reduct $\psi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n, \overline{y}_1, \dots, \overline{y}_{m'})$ of $\psi(\overline{x}, \overline{y})$ where $\overline{y}_i \coloneqq (y_{i,1}, \dots, y_{i,t})$ for all $i \in [1, m']$. Using this Θ-reduct, we let

$$\begin{aligned}\varphi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n) \;\coloneqq\; (\mathsf{Q}{+}k)(\overline{y}_1, \dots, \overline{y}_{m'})\Big(&\bigwedge_{i=1}^{m'} \theta(\overline{y}_i) \;\wedge \\ &\psi^{-\Theta}(\overline{x}_1, \dots, \overline{x}_n, \overline{y}_1, \dots, \overline{y}_{m'})\Big).\end{aligned}$$

By construction, $\varphi^{-\Theta}(\overline{x}_1,\dots,\overline{x}_n)$ belongs to $\mathsf{L}_{\mathrm{tpl}}[\sigma]$.

To see that Statement (i) of Claim 1 is satisfied, consider a σ-structure $\mathcal{A}$ for which $\Theta[\mathcal{A}]$ is defined. Furthermore, let $\overline{b}_1,\dots,\overline{b}_n$ be elements from the universe of $\Theta[\mathcal{A}]$. Due to the definition of the universe of $\Theta[\mathcal{A}]$ and since $\psi^{-\Theta}(\overline{x}_1,\dots,\overline{x}_n,\overline{y}_1,\dots,\overline{y}_{m'})$ is a Θ-reduct of $\psi(\overline{x},\overline{y})$, the following equivalence holds for all tuples $\overline{c}_1,\dots,\overline{c}_{m'}$ from A^t:

$$\begin{array}{ll} & \overline{c}_1,\dots,\overline{c}_{m'} \text{ are from the universe of } \Theta[\mathcal{A}] \quad \text{and} \\ & \Theta[\mathcal{A}] \ \models\ \psi[\overline{b}_1;\dots;\overline{b}_n;\overline{c}_1;\dots;\overline{c}_{m'}] \\ \text{iff} & \mathcal{A} \models \theta[\overline{c}_i] \text{ for all } i\in[1,m'] \quad \text{and} \quad \mathcal{A}\ \models\ \psi^{-\Theta}[\overline{b}_1,\dots,\overline{b}_n,\overline{c}_1,\dots,\overline{c}_{m'}]. \end{array}$$

Thus, it follows from the construction of $\varphi^{-\Theta}(\overline{x}_1,\dots,\overline{x}_n)$ that

$$\begin{array}{rrcl} & \Theta[\mathcal{A}] & \models & \varphi[\overline{b}_1;\dots;\overline{b}_n] \\ \text{iff} & \mathcal{A} & \models & \varphi^{-\Theta}[\overline{b}_1,\dots,\overline{b}_n]. \end{array}$$

By Statements (ii) to (iv) of Claim 1, the formula $\psi^{-\Theta}(\overline{x}_1,\dots,\overline{x}_n,\overline{y}_1,\dots,\overline{y}_{m'})$ has quantifier rank $\leq t\cdot(q{-}m')+q_\Theta$ and dimension $\leq t\cdot m$. Furthermore, if $\psi(\overline{x},\overline{y})$ is from $\mathsf{FO}{+}\mathrm{unM}_{\mathrm{tpl}}[\tau]$, then its Θ-reduct has the same threshold and maximum period.

Thus, it is straightforward to see that $\varphi^{-\Theta}(\overline{x}_1,\dots,\overline{x}_n)$ has quantifier rank

$$\leq\ t\cdot m' + t\cdot(q{-}m') + q_\Theta \ =\ t\cdot q + q_\Theta,$$

dimension $\leq t\cdot m$, and, if $\varphi(\overline{x})$ belongs to $\mathsf{FO}{+}\mathrm{unM}_{\mathrm{tpl}}[\tau]$, the same threshold and maximum period as $\varphi(\overline{x})$. Therefore, Statements (ii) to (iv) of Claim 1 are satisfied.

Time complexity. In the following, we show that also Statement (v) of Claim 1 holds for the particular case of an ultimately periodic logic L.

For an *atomic formula* φ, clearly, there is a number $c\in\mathbb{N}_{\geq 1}$ such that $\varphi^{-\Theta}$ can be constructed in $\leq c\cdot||\Theta||\cdot||\varphi||$ time steps.

In the case of φ being a *Boolean combination* it is also straightforward to see that $\varphi^{-\Theta}$ can be computed in at most $c\cdot||\Theta||\cdot||\varphi||$ time steps by calling the algorithm recursively on the subformulae.

If φ is a *quantified formula*, that is, of the shape $\varphi=(\mathsf{Q}{+}k)\overline{y}\,\psi$, the algorithm takes at most $c\cdot||\Theta||\cdot||\psi||$ time steps to compute the Θ-reduct for ψ. By the shape of $\varphi^{-\Theta}$ one can verify that it can be constructed in at most

$$\begin{array}{lll} & c'\cdot(||(\mathsf{Q}{+}k)|| + m'\cdot(t+||\theta||)) + c\cdot||\Theta||\cdot||\psi|| & \\ < & 2c'\cdot(||\varphi||-||\psi||)\cdot||\Theta|| + c\cdot||\Theta||\cdot||\psi|| & \leq \quad c\cdot||\Theta||\cdot||\varphi|| \end{array}$$

time steps, for $c \geq 2c'$.

In particular, this implies that $\varphi^{-\Theta}$ has size in $||\Theta|| \cdot \mathcal{O}(||\varphi||)$. It follows that, altogether, the construction of a Θ-reduct for φ from Θ and φ takes time in

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + ||\Theta|| \cdot \mathcal{O}(||\varphi||).$$

This completes the proof of Lemma 2.6.4. □

2.7 Graphs

In this section, we recall standard notation on graphs (cf., e.g., [EF99]) and describe a sequence of slow-growing first-order formulae that recognise paths in graphs up to a certain length. From now on, E will always denote a binary relation symbol. A *graph* $\mathcal{A}$ is a structure over the signature (E). We also call the elements of the universe of $\mathcal{A}$ *nodes*, and the tuples of the relation $E^{\mathcal{A}}$ *edges*. The graph $\mathcal{A}$ is *undirected* if for all $(a,b) \in E^{\mathcal{A}}$, also $(b,a) \in E^{\mathcal{A}}$, and it is *loop-free* if $(a,a) \notin E^{\mathcal{A}}$ for all $a \in A$.[2]

The *degree of a node* $a \in A$ is the number of distinct $b \in A$ for which $(a,b) \in E^{\mathcal{A}}$ or $(b,a) \in E^{\mathcal{A}}$. The *degree of* $\mathcal{A}$ is the maximum degree of its nodes. We also say that $\mathcal{A}$ is d-bounded (for a *degree bound* $d \in \mathbb{N}$) if $\mathcal{A}$ has degree $\leq d$.

A *path* from a node a to a node b of $\mathcal{A}$ is a tuple $(a_1, \dots, a_n)$ of $n \geq 1$ nodes from A with $a_1 = a$ and $a_n = b$, such that $(a_i, a_{i+1}) \in E^{\mathcal{A}}$ for every $i \in [1, n)$. The *length* of the path $(a_1, \dots, a_n)$ is the number of edges on the path and thus $n - 1$.

The following lemma shows that paths in graphs up to length n can be defined by $\mathsf{FO}[E]$-formulae of size logarithmic in n. The construction is based on [FG04, Lemma 20]. In particular, these formulae will be useful for the proofs of the lower bounds presented in Chapter 9. However, we will also use these formulae in Section 2.8 to speak about distances and local neighbourhoods in relational structures

Lemma 2.7.1. *There is a sequence* $(\mathrm{path}_{\leq n}(x,y))_{n \geq 0}$ *of* $\mathsf{FO}[E]$*-formulae such that for every* $n \geq 0$*, the following holds for each graph* $\mathcal{A}$ *and all* $a, b \in A$*:*

$$\mathcal{A} \models \mathrm{path}_{\leq n}[a,b]$$

[2]Note that, by this definition and contrary to, e.g., [EF99], a graph is allowed to contain directed edges and loops if not explicitly described as undirected and loop-free, respectively.

iff *there is a path of length* $\leq n$ *from* a *to* b *in* $\mathcal{A}$.

Furthermore, there is an algorithm which computes the formula $\mathrm{path}_{\leq n}(x,y)$ *on input of* $n \geq 0$ *in time* $\mathcal{O}(\log n)$ *for* $n \geq 1$.

Proof. For paths of length 0 and 1, let

$$\mathrm{path}_{\leq 0}(x,y) \;\coloneqq\; x{=}y \quad \text{and} \quad \mathrm{path}_{\leq 1}(x,y) \;\coloneqq\; \mathrm{path}_{\leq 0}(x,y) \;\vee\; E(x,y).$$

For paths of length at least 2, we proceed recursively: For $n \geq 1$, let

$$\mathrm{path}_{\leq 2n}(x,y) \;\coloneqq\; \exists z \forall u \forall v \Big(\big((u{=}x \wedge v{=}z) \;\vee\; (u{=}z \wedge v{=}y) \big) \;\rightarrow\; \mathrm{path}_{\leq n}(u,v) \Big).$$

and

$$\mathrm{path}_{\leq 2n+1}(x,y) \;\coloneqq\; \exists z \left(\mathrm{path}_{\leq 1}(x,z) \;\wedge\; \mathrm{path}_{\leq 2n}(z,y) \right).$$

A straightforward induction over the path length $n \in \mathbb{N}$ leads to the upper bound on the time required for the construction of the formula. □

In Section 9.2, further notation concerning forests and trees will be introduced.

2.8 Locality

This section introduces notation concerning local neighbourhoods in structures, as used, e.g., in [EF99, Lib04]. The key concept, which we will explain first, is the Gaifman graph of a structure [Gai82]. The Gaifman graph leads to a distance measure between the elements of a structure, which allows to define local neighbourhoods around such elements. Furthermore, it allows to define structures of bounded degree by generalising the concept of graphs of bounded degree. In the remainder of the section, we will examine the properties of local neighbourhoods in structures of bounded degree that will be crucial for the algorithms described in the subsequent chapters.

For the following, we let $c_1, c_2, \ldots$ be a sequence of pairwise distinct constant symbols and we let $\sigma \coloneqq (R_1, \ldots, R_k, c_1, \ldots, c_\ell)$ be a signature with $k \geq 0$ relation symbols R_i of arity $r_i \geq 1$, for $i \in [1,k]$, and $\ell \geq 0$ constant symbols.

$\mathcal{A} :=$

$R^{\mathcal{A}}$		
a	b	c
d	a	d
e	f	f

$P^{\mathcal{A}}$
a
d
e

$\mathcal{G}_{\mathcal{A}} :=$

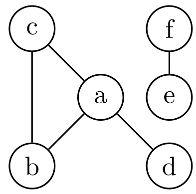

Figure 2.1 A structure $\mathcal{A}$ over the signature (R, P) and its Gaifman graph $\mathcal{G}_{\mathcal{A}}$.

2.8.1 Gaifman Graph

The *Gaifman graph* $\mathcal{G}_{\mathcal{A}}$ of a σ-structure $\mathcal{A}$ is the undirected and loop-free graph with node set A and where for all distinct $a, b \in A$,

there is an edge between a and b in $\mathcal{G}_{\mathcal{A}}$

iff there is an $i \in [1, k]$ and a tuple $(a_1, \ldots, a_{r_i}) \in R_i^{\mathcal{A}}$ with $a, b \in \{a_1, \ldots, a_{r_i}\}$.

Example 2.8.1. An example for the Gaifman graph of a structure $\mathcal{A}$ over the signature $\tau := (R, P)$, where R is a ternary relation symbol and P is unary relation symbol, is depicted in Figure 2.1. Note that the unary relation $P^{\mathcal{A}}$ does not contribute to the Gaifman graph $\mathcal{G}_{\mathcal{A}}$.

We say that a σ-structure $\mathcal{A}$ is *d-bounded* (for a *degree bound* $d \in \mathbb{N}$) if its Gaifman graph $\mathcal{G}_{\mathcal{A}}$ is d-bounded. Note that, since we only consider finite structures, every σ-structure clearly is d-bounded for $d = |A| - 1$.

By $\mathfrak{C}^{d,\sigma}$ we denote the *class of all d-bounded σ-structures.* For a relational signature σ, i.e., if $\ell = 0$, we call two formulae φ, ψ of some logic $\mathsf{L}[\sigma]$ *d-equivalent*, if they are $\mathfrak{C}^{d,\sigma}$-equivalent.

Example 2.8.2. The τ-structure $\mathcal{A}$ depicted in Figure 2.1 is 3-bounded.

The *distance* $\mathrm{dist}^{\mathcal{A}}(a, b)$ between two elements a, b in a σ-structure $\mathcal{A}$ is the length of a shortest path between a and b in the Gaifman graph $\mathcal{G}_{\mathcal{A}}$, or $\mathrm{dist}^{\mathcal{A}}(a, b) := \infty$ if no such path exists. A subset $B \subseteq A$ of the universe A of a σ-structure $\mathcal{A}$ is called *s-scattered* for an $s \in \mathbb{N}$, if its elements have pairwise distance $> s$ in $\mathcal{A}$.

Example 2.8.3. Consider the unary transduction $\Theta := (\theta, \theta_E)$ from σ to (E), defined by $\theta(x) := x{=}x$ and

$$\theta_E(x, y) \;:=\; \neg x{=}y \;\wedge\; \bigvee_{i=1}^{k} \exists z_1 \cdots \exists z_{r_i} \Big(R_i(z_1, \ldots, z_{r_i}) \wedge \bigvee_{i=1}^{r_i} x{=}z_i \wedge \bigvee_{i=1}^{r_i} y{=}z_i \Big).$$

Note that Θ has size in $\mathcal{O}(||\sigma||)$ and that $\Theta[\mathcal{A}] = \mathcal{G}_{\mathcal{A}}$ for each σ-structure $\mathcal{A}$.

By using Lemma 2.6.4 to construct Θ-reducts for the formulae $(\mathrm{path}_{\leq n}(x,y))_{n\geq 0}$ from Lemma 2.7.1, we obtain the following corollary.

Corollary 2.8.4. *There is a sequence* $(\mathrm{dist}_{\leq n}(x,y))_{n\geq 0}$ *of* $\mathsf{FO}[\sigma]$*-formulae such that for all* $n \geq 0$ *the following holds for each* σ*-structure* $\mathcal{A}$ *and all* $a, b \in A$*:*

$$\mathcal{A} \models \mathrm{dist}_{\leq n}[a,b] \quad \textit{iff} \quad \mathrm{dist}^{\mathcal{A}}(a,b) \leq n.$$

Furthermore, there is an algorithm which computes the formula $\mathrm{dist}_{\leq n}(x,y)$ *on input of* σ *and* $n \geq 0$ *in time* $||\sigma|| \cdot \mathcal{O}(\log n)$ *for* $n \geq 1$*.*

For a better readability, we will also write $\mathrm{dist}(x,y) \leq n$ for the formula $\mathrm{dist}_{\leq n}(x,y)$. Moreover, if $\overline{x}$ is a tuple $(x_1, \ldots, x_m)$ of $m \geq 1$ pairwise variables, we write $\mathrm{dist}(\overline{x}, y) \leq n$ for the formula $\bigvee_{i=1}^{m} \mathrm{dist}(x_i, y) \leq n$.

2.8.2 Neighbourhoods

Consider a σ-structure $\mathcal{A}$. For each $r \geq 0$ and every $a \in A$, the *r-neighbourhood of a in $\mathcal{A}$* is the set

$$N_r^{\mathcal{A}}(a) \;\coloneqq\; \{b \in A \,:\, \mathrm{dist}^{\mathcal{A}}(a,b) \leq r\}.$$

For a set $W \subseteq A$ we let $N_r^{\mathcal{A}}(W) \coloneqq \bigcup_{a\in A} N_r^{\mathcal{A}}(a)$. Furthermore, for a non-empty tuple $\overline{a} = (a_1, \ldots, a_n)$ of elements from A, we write $N_r^{\mathcal{A}}(\overline{a})$ for $N_r^{\mathcal{A}}(\{a_1, \ldots, a_n\})$.

2.8.3 Types and Spheres

For each $r \geq 0$ and every $n \geq 1$, a *σ-type with n centres and radius r* is a structure $\tau = (\mathcal{B}, b_1, \ldots, b_n)$ over the signature $(R_1, \ldots, R_k, c_1, \ldots, c_n)$, where $\mathcal{B}$ is a structure of signature $(R_1, \ldots, R_k)$ and $(b_1, \ldots, b_n) \in B^n$ is a tuple with the property that all elements in the universe of $\mathcal{B}$ have distance $\leq r$ to at least one of the elements $b_1, \ldots, b_n$. In other words, $B = N_r^{\mathcal{B}}(b_1, \ldots, b_n)$. We also call the elements $b_1, \ldots, b_n$ the *centres* of τ. If the signature, the radius, and the number of centres are understood from the context, we will sometimes omit them and just speak of a type.

For each σ-structure $\mathcal{A}$ and every tuple $(a_1, \ldots, a_n) \in A^n$, the *$r$-sphere of $(a_1, \ldots, a_n)$ in $\mathcal{A}$* is the type

$$\mathcal{N}_r^{\mathcal{A}}(a_1, \ldots, a_n) \;\coloneqq\; (\mathcal{A}_{|(R_1,\ldots,R_k)}[N_r^{\mathcal{A}}(a_1, \ldots, a_n)], a_1, \ldots, a_n).$$

Example 2.8.5. Reconsider the structure $\mathcal{A}$ over the signature (R, P) from Example 2.8.1, depicted in Figure 2.1. The 1-sphere of the tuple (b, f) is the (R, P, c_1, c_2)-structure $(\mathcal{B}, b, f)$ where $\mathcal{B}$ is the substructure of $\mathcal{A}$ induced by the elements a, b, c, e, f, that is, the (R, P)-structure with $R^{\mathcal{B}} := \{(a, b, c), (e, f, f)\}$ and $P^{\mathcal{B}} := \{a, e\}$.

For a σ-type τ with n centres and radius r, we say that the tuple $(a_1, \ldots, a_n)$ *realises* τ if, and only if,

$$\mathcal{N}_r^{\mathcal{A}}(a_1, \ldots, a_n) \;\cong\; \tau.$$

For a σ-type τ with *one* centre and radius r and a σ-structure $\mathcal{A}$, we furthermore denote by

$$\tau(\mathcal{A}) \;:=\; \{a \in A \,:\, \mathcal{N}_r^{\mathcal{A}}(a) \cong \tau\}$$

the *set of elements of* $\mathcal{A}$ *that realise* τ.

2.8.4 Types in Structures of Bounded Degree

Let $d \geq 0$ be a degree bound. The crucial property of d-bounded structures, used along the course of this thesis is that there is an upper bound on the size of d-bounded types realised in a d-bounded structure, which only depends on the their radius, number of centres, and the degree bound, but not on the size of the whole structure.

To bound the size of a d-bounded σ-type with a single centre in dependence from its radius $r \geq 0$, let $\nu_d \colon \mathbb{N} \to \mathbb{N}_{\geq 1}$ be defined by

$$\nu_d(r) \;:=\; 1 + d \cdot \sum_{i=0}^{r-1} (d-1)^i.$$

Then, for any d-bounded σ-structure $\mathcal{A}$, any element $a \in A$, and any $r \geq 0$, we have

$$|N_r^{\mathcal{A}}(a)| \;\leq\; \nu_d(r)\,.$$

Observe that for all $r \geq 0$, we have $\nu_0(r) = 1$ and $\nu_1(r) \leq 2$. On the other hand,

$$\nu_2(r) \;=\; 2r + 1$$

and, for degree bounds $d \geq 3$,

$$(d-1)^r \;\leq\; \nu_d(r) \;\leq\; d^{r+1}.$$

In other words, ν_d is growing linearly for $d \leq 2$ and exponentially for $d \geq 3$.

Two σ-types can be checked for isomorphism by a straightforward brute-force algorithm. For d-bounded σ-types, we obtain the following upper bound on the time complexity of such an algorithm.

Lemma 2.8.6. *There is an algorithm which, on input of a signature σ and two σ-types τ and τ' with $n \geq 1$ centres decides whether $\tau \cong \tau'$. The algorithm takes time in*

$$2^{\mathcal{O}(||\sigma||)\cdot(n\cdot\nu_d(r))^2},$$

where $d, r \geq 0$ are upper bounds on the degree bound and the radius of τ and τ'.

Proof. Let σ be a signature, and let τ and τ' be two σ-types with $n \geq 1$ centres. Let $d, r \geq 0$ such that τ and τ' are both d-bounded and of radius $\leq r$. Let $N := n \cdot \nu_d(r)$ be an upper bound on the size of the universes of τ and τ'.

For the special case of $N = 1$, there is only one bijection mapping the single element of τ to the single element of τ', and it takes time in $\mathcal{O}(||\sigma||)$, to check whether this bijection is an isomorphism.

If $N \geq 2$, then for every bijection between the elements of τ and τ', it can be checked in at most $c' \cdot (n + N^{||\sigma||}) \leq N^{c''\cdot||\sigma||}$ time steps, for numbers $c', c'' \in \mathbb{N}_{\geq 1}$ with $c' < c''$, whether the bijection is indeed an isomorphism. Since there are at most N^N bijections, the test whether τ and τ' are isomorphic can be performed in time

$$N^N \cdot N^{\mathcal{O}(||\sigma||)} \quad \subseteq \quad 2^{\mathcal{O}(||\sigma||)\cdot N^2}.$$

Thus, in any case, the algorithm takes time in $2^{\mathcal{O}(||\sigma||)\cdot(n\cdot\nu_d(r))^2}$. $\square$

The upper bound $n \cdot \nu_d(r)$ on the number of elements in d-bounded σ-types of radius $r \geq 0$ and with $n \geq 1$ centres implies that there is also only a finite number of such types that are pairwise non-isomorphic. In fact, this number grows 2-fold exponentially with the radius.

In the remainder of this section, we can suppose σ to be relational. For $d, r \geq 0$ and $n \geq 1$, we denote by $\mathfrak{T}_r^{d,\sigma}(n)$ a *set of representatives of the isomorphism classes of all d-bounded σ-types with n centres and radius r.* That is, for every d-bounded type τ with n centres and radius r that may be realised by a tuple $\overline{a} \in A^n$ in a d-bounded σ-structure $\mathcal{A}$, there is precisely one type $\tau' \in \mathfrak{T}_r^{d,\sigma}(n)$ with $\tau \cong \tau'$. The following lemma uses the isomorphism test of Lemma 2.8.6 to construct such sets $\mathfrak{T}_r^{d,\sigma}(n)$.

Lemma 2.8.7. *There is an algorithm which, on input of a relational signature σ, $d, r \geq 0$, and $n \geq 1$, computes the set $\mathfrak{T}_r^{d,\sigma}(n)$ in time*

$$2^{\max\{2, n \cdot \nu_d(r)\}^{\mathcal{O}(||\sigma||)}}.$$

Proof. Let σ be a relational signature, let $d, r \geq 0$, and let $n \geq 1$. Recall that the universe of each type in the set $\mathfrak{T}_r^{d,\sigma}(n)$ has at most $N := n \cdot \nu_d(r)$ elements.

For the case that $N = 1$, there are at most $2^{||\sigma||}$ types in $\mathfrak{T}_0^{d,\sigma}(1)$ which can be easily constructed in time $\mathcal{O}(2^{||\sigma||}) \subseteq 2^{2^{\mathcal{O}(||\sigma||)}}$.

In the following, we suppose that $N \geq 2$ and let the universe of each type in $\mathfrak{T}_r^{d,\sigma}(n)$ be a subset of $[1, N]$. Hence, the relations of an arbitrary type in $\mathfrak{T}_r^{d,\sigma}(n)$ can be represented by a word over the alphabet $\{0, 1\}$ of length at most $N^{||\sigma||}$. Furthermore, each of its n centres is interpreted by an element from $[1, N]$. Hence, there are at most

$$N^n \cdot 2^{N^{||\sigma||}} \quad \leq \quad 2^{N \cdot \log N + N^{||\sigma||}} \quad < \quad 2^{N^{||\sigma||+2}}$$

candidates for types in $\mathfrak{T}_r^{d,\sigma}(n)$.

For any such candidate, we need at most time $N^{\mathcal{O}(||\sigma||)}$ to decide whether the candidate is indeed a d-bounded σ-type with radius r. For any two such candidates, we use the algorithm from Lemma 2.8.6 for testing whether they are isomorphic. In summary, $\mathfrak{T}_r^{d,\sigma}(n)$ can be constructed in time

$$2^{N^{||\sigma||+2}} \cdot N^{\mathcal{O}(||\sigma||)} + \left(2^{N^{||\sigma||+2}}\right)^2 \cdot 2^{\mathcal{O}(||\sigma||) \cdot N^2} \quad \subseteq \quad 2^{N^{\mathcal{O}(||\sigma||)}}.$$

Thus, we can subsume the cases of $N = 1$ and $N \geq 2$ under the upper bound stated in the lemma. $\square$

For a d-bounded σ-type τ with radius r and n centres, one can construct [BK12] a *sphere-formula* $\mathrm{sph}_\tau(\overline{x})$ with the free variables $\overline{x} = (x_1, \ldots, x_n)$ from $\mathsf{FO}[\sigma]$, such that for every σ-structure $\mathcal{A}$ and each tuple $\overline{a} \in A^n$,

$$\mathcal{A} \models \mathrm{sph}_\tau[\overline{a}] \quad \text{iff} \quad \mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \tau.$$

The following lemma gives an upper bound on the time needed to construct such a sphere-formulae.

Lemma 2.8.8. *There is an algorithm which, on input of a relational signature σ and, for a degree bound $d \geq 0$, a d-bounded σ-type τ with radius $r \geq 0$ and $n \geq 1$ centres, computes the formula $\mathrm{sph}_\tau(\overline{x})$ in time*

$$\max\{2, n \cdot \nu_d(r)\}^{\mathcal{O}(||\sigma||)}.$$

Proof. Suppose that $\sigma = (R_1, \ldots, R_k)$ for some $k \geq 0$. Let $\tau = (\mathcal{A}, c_1, \ldots, c_n)$, let $M := |A|$, and let $\{a_1, \ldots, a_M\} = A$. Choose indices $i_1, \ldots, i_n \in [1, M]$ such that $c_j = a_{i_j}$ for all $i \in [1, n]$. With this preparation, we can choose

$$\begin{aligned} \mathrm{sph}_\tau(\overline{x}) \;:=\; \quad & \exists z_1 \cdots \exists z_M \Big(\bigwedge_{\varphi \in \Phi} \varphi(z_1, \ldots, z_M) \;\wedge\; \bigwedge_{j=1}^{n} x_j{=}z_{i_j} \\ & \wedge\; \forall y \big(\mathrm{dist}(\overline{x}, y) \leq r \;\rightarrow\; \bigvee_{i=1}^{M} y{=}z_i\big)\Big) \end{aligned}$$

where Φ is the set of all atomic and negated atomic formulae $\varphi(z_1, \ldots, z_M)$ over the signature σ such that $\mathcal{A} \models \varphi[a_1, \ldots, a_M]$.

Let $N := n{\cdot}\nu_d(r)$. The cardinality of the set Φ is in $\mathcal{O}(k)$ if $N = 1$ and, if $N \geq 2$, in $N^{\mathcal{O}(||\sigma||)}$. Hence, the formula $\mathrm{sph}_\tau(\overline{x})$ can be constructed in time $\mathcal{O}(||\sigma||)$ if $N = 1$, and in time $N^{\mathcal{O}(||\sigma||)}$ if $N \geq 2$. Altogether, we can bound the time required for the construction of $\mathrm{sph}_\tau(\overline{x})$ by the expression stated in the lemma. $\square$

2.9 A Divide-and-Conquer Scheme for Formulae

Suppose that σ is a signature, that M is a finite and non-empty set, and that $\varphi_j(y)$ for $j \in M$ are formulae with the property that each element in any σ-structure satisfies at most one of these formulae. To check whether the number of elements in a σ-structure that satisfy one of these formulae is congruent r modulo p for some $p \geq 2$ and $r \in [0, p)$, or exceeds a certain threshold $k \geq 0$, we clearly can use the formulae

$$\exists^{\equiv r \bmod p} y \bigvee_{j \in M} \varphi_j(y) \tag{2.1}$$

and

$$\exists^{>k} y \bigvee_{j \in M} \varphi_j(y), \tag{2.2}$$

respectively. A reoccuring task in the following chapters (in particular in Section 3.2, Section 6.2, and Section 7.2) will be, to decompose formulae similar to Sentence (2.1) and Sentence (2.2) into Boolean combinations of formulae that count the elements satisfying each of the formulae $\varphi_j(y)$, $j \in M$, *separately.* In the particular case of Sentence (2.1) and Sentence (2.2), a first straightforward attempt gives us the sentence

$$\bigvee_{f \in F} \bigwedge_{j \in M} \exists^{\equiv f(j) \bmod p} y\, \varphi_j(y), \tag{2.3}$$

where F is the set of all functions $f\colon M \to [0,p)$ such that the sum of $f(j)$ for all $j \in M$ is congruent to r modulo p, and the sentence

$$\bigvee_{g\in G}\ \bigwedge_{\substack{j\in M,\\ g(j)\geq 0}} \exists^{>g(j)} y\, \varphi_j(y),$$

where G is the set of all functions $g\colon M \to [-1,k]$ such that the sum of $g(j)+1$ for all $j \in M$ equals $k+1$. The disadvantage of these latter formulae is that already the number of clauses of their corresponding outer disjunction grows exponentially with the cardinality of the set M. In particular, $|F| = p^{|M|-1}$.

Example 2.9.1. Let σ be a relational signature, let $d \geq 0$ be a degree bound, and let $r \geq 0$. Each element of a d-bounded σ-structure $\mathcal{A}$ realises precisely one of the σ-types in $\mathfrak{T}_r^{d,\sigma}(1)$, that is, it satisfies precisely one of the formulae $\mathrm{sph}_\tau(y)$ for $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$. Expressing the statement *"$\mathcal{A}$ has a universe of even cardinality"* in the manner of Sentence (2.3) results in a sentence of size $> 2^{|\mathfrak{T}_r^{d,\sigma}(1)|}$.

In this section, we describe a divide-and-conquer approach, which leads to an exponentially smaller size of the resulting Boolean combinations in comparison to the naive brute-force approach just described. More precisely, the size of the resulting Boolean combination only grows polynomially with $|M|$ instead of exponentially. In particular, in Section 3.2, this will help us to obtain an algorithm whose running time meets the corresponding lower bounds, and in Section 6.2 it will reduce the gap between upper and lower bounds. The approach distills the idea of constructions used in [HHS15, HKS16].

The following two lemmas describe the divide-and-conquer procedure for the cases of modulo-counting and threshold-counting. Both lemmas are stated in a very general way which is necessary to cover the various settings in the subsequent chapters in which they are used. Note that the restriction to ultimately periodic logics is not necessary for the constructions themselves, but only for their statement and analysis as algorithms.

Lemma 2.9.2. *Let L be an ultimately periodic logic. There is an algorithm which, on input of*

- *numbers $p \geq 2$ and $r \in [0,p)$,*
- *a non-empty and finite set M, and*
- *L-formulae δ_j^i for all $i \in [0,p)$ and $j \in M$,*

computes an L*-formula* $\langle \delta^i_j \rangle^{\equiv r \bmod p}_M$ *that is equivalent to the* L*-formula*

$$\bigvee_{f \in F} \bigwedge_{j \in M} \delta^{f(j)}_j, \tag{2.4}$$

where F *is the set of all functions* $f \colon M \to [0,p)$ *such that the sum of* $f(j)$ *for all* $j \in M$ *is congruent to* r *modulo* p*.*

The algorithm takes time in

$$(2p)^{\lceil \log |M| \rceil + 1} \cdot \mathcal{O}(n),$$

where $n \geq 1$ *is an upper bound on the size of* δ^i_j *for all* $i \in [0,p)$ *and* $j \in M$*.*

Note that Formula (2.4) has size in $p^{|M|-1} \cdot |M| \cdot \mathcal{O}(n)$, that is, the formula grows exponentially with the size of M. On the other hand, the formula $\langle \delta^i_j \rangle^{\equiv r \bmod p}_M$ only grows polynomially with the size of M.

Proof. Let L be an ultimately periodic logic. Let $p \geq 2$, $r \in [0,p)$, let M be a non-empty and finite set, and let δ^i_j for all $i \in [0,p)$ and $j \in M$ be an L-formula.

The construction proceeds by a divide-and-conquer approach on the set M.

For each singleton set $\{m\} \subseteq M$ *and each* $s \in [0,p)$, let

$$\langle \delta^i_j \rangle^{\equiv s \bmod p}_{\{m\}} \quad := \quad \delta^s_m.$$

For any subset $M' \subseteq M$ *of cardinality* $|M'| \geq 2$ *and each* $s \in [0,p)$, we divide M' into two sets of almost equal size. More precisely, we choose $M_1 \subset M'$ with $|M_1| = \lfloor |M'|/2 \rfloor$, let $M_2 = M' \setminus M_1$, and let the expression

$$\langle \delta^i_j \rangle^{\equiv s \bmod p}_{M'}$$

denote the disjunction of all formulae

$$\langle \delta^i_j \rangle^{\equiv s_1 \bmod p}_{M_1} \quad \wedge \quad \langle \delta^i_j \rangle^{\equiv s_2 \bmod p}_{M_2}$$

where $s_1, s_2 \in [0,p)$ such that $s_1 + s_2 \equiv s \mod p$.

A straightforward induction shows that the formula $\langle \delta^i_j \rangle^{\equiv r \bmod p}_M$ is indeed equivalent to Formula (2.4): The induction base for a singleton set $\{m\} \subseteq M$ and a remainder $s \in [0,p)$ follows directly from the construction of $\langle \delta^i_j \rangle^{\equiv s \bmod p}_{\{m\}}$, since, of course, there is only one function $f \colon \{m\} \to [0,p)$ such that $f(m) \equiv s \mod p$. For a subset $M' \subseteq M$ of cardinality ≥ 2, the subsets M_1, M_2 of M'

defined above, and a remainder $s \in [0,p)$, the formula $\langle \delta^i_j \rangle^{\equiv s \bmod p}_{M'}$ is equivalent to the disjunction of all formulae

$$\bigvee_{f_1 \in F_1} \bigwedge_{j \in M_1} \delta_j^{f_1(j)} \quad \vee \quad \bigvee_{f_2 \in F_2} \bigwedge_{j \in M_2} \delta_j^{f_2(j)} \tag{1}$$

for all $s_1, s_2 \in [0,p)$ such that $s_1 + s_2 \equiv s \mod p$ and such that, for each $k \in \{1,2\}$, F_k is the set of all functions $f\colon M_k \to [0,p)$ where the sum of $f(j)$ for all $j \in M_k$ is congruent to s_k modulo p. In every clause of the disjunction, for all $f_1 \in F_1$ and $f_2 \in F_2$, the sum of the values $f_k(j)$ for all $k \in \{1,2\}$ and $j \in M_k$ is congruent to s modulo p. On the other hand, the range of every function $f\colon M' \to [0,p)$ where the sum of $f(j)$ for all $j \in M'$ is congruent to s modulo p can be partitioned into the sets M_1 and M_2, leading to functions $f_k\colon M_k \to [0,p)$, for $k \in \{1,2\}$, such that the sum of $f_k(j)$ for all $j \in M_k$ is congruent s_k for values $s_1, s_2 \in [0,p)$ with $s_1 + s_2 \equiv s \mod p$. Thus, Formula (1) is equivalent to the formula

$$\bigvee_{f \in F} \bigwedge_{j \in M'} \delta_j^{f(j)}$$

where F is the set of all functions $f\colon M' \to [0,p)$ for which the sum of $f(j)$ for all $j \in M'$ is congruent to s modulo p.

Time complexity. For an upper bound on the time required to construct the formula $\langle \delta^i_j \rangle^{\equiv r \bmod p}_{M}$, observe that the recursion depth of the construction is at most $\lceil \log |M| \rceil + 1$. Furthermore, each recursive call for the non-singleton sets $M' \subseteq M$ involves $2p$ subsequent recursive calls. On the other hand, for singleton sets M', the constructed formula has size $\leq n$, where $n \geq 1$ is an upper bound on the size of the formulae δ^i_j for all $i \in [0,p)$ and $j \in M$. Thus, the formula $\langle \varphi^i_j \rangle^{\equiv r \bmod p}_{M}$ can altogether be constructed within the time bound stated in the lemma. $\square$

Example 2.9.3. Continuing with Example 2.9.1, the statement *"$\mathcal{A}$ has a universe of even cardinality"* can now be expressed by the sentence

$$\langle \delta^i_\tau \rangle^{\equiv 0 \bmod 2}_{\mathfrak{T}^{d,\sigma}_r(1)}$$

with $\delta^i_\tau := \exists^{\equiv i \bmod 2} y \; \mathrm{sph}_\tau(y)$ for all $i \in \{0,1\}$ and $\tau \in \mathfrak{T}^{d,\sigma}_r(1)$. The size of this sentence only grows polynomially with the cardinality of the set $\mathfrak{T}^{d,\sigma}_r(1)$.

The following lemma is proven in a similar way to Lemma 2.9.2.

Lemma 2.9.4. *Let* L *be an ultimately periodic logic. There is an algorithm which, on input of*

- *a number* $k \geq 0$,
- *a non-empty and finite set* M, *and*
- L*-formulae* δ_j^i *for all* $i \in [0, k]$ *and* $j \in M$,

computes an L*-formula* $\langle \delta_j^i \rangle_M^{>k}$ *that is equivalent to the* L*-formula*

$$\bigvee_{g \in G} \bigwedge_{\substack{j \in M, \\ g(j) \geq 0}} \delta_j^{g(j)}, \tag{2.5}$$

where G *is the set of all functions* $g \colon M \to [-1, k]$ *such that the sum of* $g(j) + 1$ *for all* $j \in M$ *equals* $k + 1$.

The algorithm takes time in

$$(2k{+}2)^{\lceil \log |M| \rceil + 1} \cdot \mathcal{O}(n),$$

where $n \geq 1$ *is an upper bound on the size of* δ_j^i *for all* $i \in [0, k]$ *and* $j \in M$.

Proof. Let L be an ultimately periodic logic. Let $k \geq 0$, let M be a non-empty and finite set, and let δ_j^i for all $i \in [0, p)$ and $j \in M$ be an L-formula. Again, the construction proceeds by a divide-and-conquer approach on the set M.

For each singleton set $\{m\} \subseteq M$ *and each* $\ell \in [0, k]$, let

$$\langle \delta_j^i \rangle_{\{m\}}^{>\ell} \quad := \quad \delta_m^\ell.$$

For any subset $M' \subseteq M$ *of cardinality* $|M'| \geq 2$ *and each* $\ell \in [0, k]$, we divide M' into two sets M_1, M_2 of almost equal size, and let the expression

$$\langle \delta_j^i \rangle_{M'}^{>\ell}$$

denote the disjunction of the formula $\langle \delta_j^i \rangle_{M_1}^{>\ell} \;\vee\; \langle \delta_j^i \rangle_{M_2}^{>\ell}$ with all formulae

$$\langle \delta_j^i \rangle_{M_1}^{>\ell_1} \quad \wedge \quad \langle \delta_j^i \rangle_{M_2}^{>\ell_2}$$

where $\ell_1, \ell_2 \in [0, \ell)$ and $(\ell_1{+}1) + (\ell_2{+}1) = \ell + 1$.

A straightforward induction as in the proof of Lemma 2.9.2 shows that the formula $\langle \delta_j^i \rangle_M^{>k}$ is equivalent to Formula (2.5).

Time complexity. For an upper bound on the time required to construct the formula $\langle \delta^i_j \rangle^{>k}_M$, we proceed in a similar fashion as in the case of modulo-counting quantifiers. The recursion depth of the construction is at most $\lceil \log |M| \rceil + 1$ and each recursive call for the non-singleton sets $M' \subseteq M$ involves at most $2k+2$ further recursive calls. Thus, the formula $\langle \delta^i_j \rangle^{>k}_M$ can altogether be constructed within the time bound stated in the lemma. $\square$

3 Hanf Normal Form

This chapter is based on [HKS16]. It generalises the notion of Hanf normal form [BK12] to extensions of first-order logic by unary counting quantifiers and shows that, for formulae with modulo-counting quantifiers, such Hanf normal forms can be computed within worst-case optimal 3-fold exponential time for degree bounds $d \geq 3$. As an application, Seese's well-known algorithm for model-checking with linear data complexity on classes of structures of bounded degree [See96] will be generalised to formulae with modulo-counting quantifiers. As a second application, we obtain an alternative proof of Nurmonen's locality theorem [Nur00].

3.1 Introduction

In this chapter, we focus on Hanf's theorem [Han65] and the local normal form derived from it, called *Hanf normal form* [BK12]. Hanf's theorem was originally stated for finite and infinite structures, and later adapted to the setting of finite structures [FSV95]. Given a quantifier rank $q \geq 0$, Hanf's theorem provides conditions on the number of realisations of one-centred types of radius r (where r grows exponentially with q) in two structures that make those structures indistinguishable for an FO-sentence up to quantifier rank q.

We recapitulate Hanf's theorem for the particular case of structures of bounded degree. For the following, let σ denote a relational signature. Furthermore, recall that $\mathfrak{T}_r^{d,\sigma}(n)$ denotes a set of representatives of the isomorphism classes of all σ-types with $n \geq 1$ centres and radius $r \geq 0$ that may be realised in a d-bounded σ-structure, and that $\tau(\mathcal{A})$ is the number of realisations of the one-centred type τ in the structure $\mathcal{A}$.

Theorem 3.1.1 (Hanf's Theorem (cf., e.g., [EF99]))**.** *Let σ be a relational signature, let $d \geq 0$ be a degree bound, and let $n, q \geq 0$. Suppose that $\mathcal{A}$ and $\mathcal{B}$ are d-bounded σ-structures and that $\overline{a} \in A^n$ and $\overline{b} \in B^n$, such that the following conditions hold for $r := 3^q$:*

(1) $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \;\cong\; \mathcal{N}_r^{\mathcal{B}}(\overline{b})$.

For every type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$,

(2) either $|\tau(\mathcal{A})| \;=\; |\tau(\mathcal{B})|$ *or* $|\tau(\mathcal{A})|, |\tau(\mathcal{B})| \;\geq\; (n{+}q) \cdot \nu_d(r)$.

Then, for each tuple $\overline{x}$ *of* n *distinct variables and every formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}[\sigma]$ *with quantifier rank* $\leq q$,

$$\mathcal{A} \;\models\; \varphi[\overline{a}] \quad \textit{iff} \quad \mathcal{B} \;\models\; \varphi[\overline{b}].$$

Hanf's locality theorem implies [BK12] that for every $\mathsf{FO}[\sigma]$-formula φ and for every degree bound $d \geq 0$, there is an $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$-formula ψ that is equivalent to φ on all σ-structures of degree $\leq d$ and that is a Boolean combination of statements of the form

> *"there are at least k elements that realise type τ",*

and

> *"the interpretation of the free variables realises type ϱ."*

In the following, we will give a formal definition of this normal form – not only for first-order logic, but for the more general case of first-order logic with unary counting quantifiers. For the beginning, we only consider formulae without free variables.

Definition 3.1.2. A *counting-formula* is a formula of the shape

$$\mathsf{Q}y \ \mathrm{sph}_\tau(\overline{x}, y),$$

where Q is a unary counting quantifier, $\overline{x}$ is a tuple of $n \geq 0$ free variables, and τ is a σ-type with radius $r \geq 0$ and $n+1$ centres. We call r the *locality radius* of the counting-formula. In particular, a *counting-sentence* is a counting-formula without free variables, that is, a counting-formula where τ has one centre and $\overline{x}$ is the empty tuple. On the other hand, a *proper counting-formula* has at least one free variable.

The counting-formula above expresses that the number of interpretations for y such that the r-sphere around $\overline{x}, y$ is isomorphic to τ, belongs to the set Q. That is, for every σ-structure $\mathcal{A}$ and every tuple $\overline{a} \in A^n$, we have

$$(\mathcal{A}, \overline{a}) \;\models\; \mathsf{Q}y \ \mathrm{sph}_\tau(\overline{x}, y) \quad \text{iff} \quad |\{b \in A \,:\, \mathcal{N}_r^{\mathcal{A}}(\overline{a}, b) \cong \tau\}| \;\in\; \mathsf{Q}.$$

Proper counting-formulae are used in the original definition of Hanf normal form [BK12] (cf., Theorem 3.1.7 and Remark 3.1.8 below), and we also need them as an intermediate step in later proofs. However, in our definition of Hanf normal form, only counting-sentences occur.

Definition 3.1.3. A *Hanf normal form sentence* (for short: a HNF-*sentence*) is a Boolean combination ψ of counting-*sentences*. We also say that ψ is in *Hanf normal form*. The *locality radius* of ψ is the maximum of the locality radii of its counting-sentences.

Observation 3.1.4. *A* HNF*-sentence from* $\mathsf{FO}{+}\mathrm{unT}[\sigma]$ *is a Boolean combination of counting-sentences of the shape* $\exists^{\geq k} y\ \mathrm{sph}_\tau(y)$ *with* $k \geq 1$*. A* HNF*-sentence from* $\mathsf{FO}{+}\mathrm{unM}[\sigma]$ *can, additionally, also use counting-sentences of the shape* $\exists^{\equiv k \bmod p} y\ \mathrm{sph}_\tau(y)$ *for* $p \geq 2$ *and* $k \in [0, p)$*. Finally, a* HNF*-sentence from* $\mathsf{FO}{+}\mathrm{unC}(C)[\sigma]$ *for some* $C \subseteq C_{\mathrm{all}}$ *is built of counting-sentences of the shape* $(\mathsf{Q}{+}k)y\ \mathrm{sph}_\tau(y)$ *with* $\mathsf{Q} \in \{\exists\} \cup C$ *and* $k \geq 0$*. Note that, for every logic* L*, the tuple-counting logic* $\mathsf{L}_{\mathrm{tpl}}$ *has the same* HNF*-sentences as* L*.*

Example 3.1.5. Let $d \geq 2$ be a degree bound and let $\mathfrak{T}$ denote the set of all types with radius 1 and one centre that may be realised in graphs over the signature (E) of degree $\leq d$. Because of the bound d on the degree, this set is clearly finite. Furthermore, let τ be the (E)-type with radius 1 and one centre, consisting of a (directed) path of length 2 with the centre being situated in its middle. Then,

$$\bigwedge_{\mathfrak{T}\setminus\{\tau\}} \neg\exists y\ \mathrm{sph}_\tau(y)$$

is a HNF-sentence that states in a graph of degree $\leq d$ that every node realises τ. Thus, it is satisfied by such a graph if the graph is a disjoint union of circles (that is, paths where the first and the last node are the same) of length ≥ 4.

The following illustrates how to use Hanf's theorem to obtain d-equivalent HNF-sentences from $\mathsf{FO}{+}\mathrm{unT}[\sigma]$ for sentences from $\mathsf{FO}[\sigma]$. Note that this construction is *not effective* since it requires a decision procedure for satisfiability of FO-sentences on finite structures of bounded degree, which is not decidable [Wil94, BK12] even for graphs.

Proposition 3.1.6 ([BK12])**.** *For every degree bound* $d \geq 0$*, every sentence from* $\mathsf{FO}[\sigma]$ *is* d*-equivalent to a* HNF*-sentence from* $\mathsf{FO}{+}\mathrm{unT}[\sigma]$*.*

Proof. Let $d \geq 0$ be a degree bound, let φ be an $\mathsf{FO}[\sigma]$-sentence with quantifier rank $q \geq 0$, let $r := 3^q$, and let $t := q \cdot \nu_d(r)$ be the threshold from Hanf's theorem.

For every d-bounded σ-structure $\mathcal{A}$, let $f_{\mathcal{A}}\colon \mathfrak{T}_r^{d,\sigma}(1) \to [0,t]$ be the function where $f_{\mathcal{A}}(\tau) \coloneqq \min\{\tau(\mathcal{A}), t\}$ for each $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$. Clearly, the set of all such functions is finite. For each $f\colon \mathfrak{T}_r^{d,\sigma}(1) \to [0,t]$, let

$$\psi_f \;\coloneqq\; \bigwedge_{\substack{\tau\in\mathfrak{T}_r^{d,\sigma}(1),\\ f(\tau)<t}} \exists^{=f(\tau)}y\ \mathrm{sph}_\tau(y) \qquad\wedge\qquad \bigwedge_{\substack{\tau\in\mathfrak{T}_r^{d,\sigma}(1),\\ f(\tau)=t}} \exists^{\geq t}y\ \mathrm{sph}_\tau(y).$$

Thus, if φ is satisfiable in d-bounded σ-structures, it is d-equivalent to the disjunction over the sentences ψ_f for all functions $f\colon \mathfrak{T}_r^{d,\sigma}(1) \to [0,t]$ for which there is a d-bounded σ-structure with $\mathcal{A} \models \varphi$ and $f_{\mathcal{A}} = f$. Otherwise, φ is d-equivalent to an arbitrary unsatisfiable HNF-sentence. $\square$

[BK12] provides a 3-fold exponential algorithm and, for degree bounds $d \geq 3$, a matching lower bound. In particular, the lower bound, which we will recapitulate in Section 9.3, also shows that our algorithmic results concerning Hanf normal form for extensions of first-order logic are worst-case optimal.

Theorem 3.1.7 ([BK12, HKS13])**.** *There is an algorithm which, on input of a degree bound $d \geq 2$, a relational signature σ, and a formula $\varphi(\overline{x})$ from $\mathsf{FO}[\sigma]$, computes a Boolean combination $\psi(\overline{x})$ of counting-formulae from $\mathsf{FO{+}unT}[\sigma]$ that is d-equivalent to φ.*

Furthermore, the algorithm constructs $\psi(\overline{x})$ in time

$$2^{(||\varphi||\cdot\nu_d(4^q))^{\mathcal{O}(||\sigma||)}}.$$

Remark 3.1.8. The actual statement of Theorem 3.1.7 in [BK12, HKS13] differs from the one given above in that the constructed Boolean combinations are formulae from FO. That is, threshold-counting quantifiers $\exists^{\geq k}x\,\varphi$ are not directly available in, but defined by the formula

$$\exists y_1 \cdots \exists y_k \left(\bigwedge_{i,j\in[1,k],i\neq j} \neg y_i{=}y_j \quad\wedge\quad \forall y \left(\bigvee_{i=1}^{k} y{=}y_i \quad\to\quad \varphi \right)\right).$$

Furthermore, the output of the algorithm of [BK12, HKS13] only fits to our definition of HNF-sentences in the case of input formulae without free variables. For input formulae with free variables, it computes a Boolean combination of counting-formulae that may also use free variables.

In our following definition of Hanf normal form for formulae with free variables, we will handle free variables in a different way, which is especially well-suited to algorithmic applications, e.g., for model-checking (see Section 3.4) and for the construction of Gaifman normal form and Feferman-Vaught style decompositions (see Chapter 4 and Chapter 5). Another advantage is that the shape of formulae in Hanf normal form parallels the conditions of Hanf's Theorem even in the presence of free variables.

In the following, we generalise Definition 3.1.3 for Hanf normal form sentences from sentences to formulae with free variables. Recall that, for a σ-type ϱ with radius $r \geq 0$ and $n \geq 1$ centres,

$$\mathcal{A} \models \mathrm{sph}_\varrho[\overline{a}] \quad \text{iff} \quad \mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \varrho.$$

The *locality radius* of a sphere-formula $\mathrm{sph}_\varrho(\overline{x})$ is the radius r of the type ϱ.

Definition 3.1.9. A *Hanf normal form formula* (for short: a HNF-*formula*) is a Boolean combination ψ of counting-*sentences* and sphere-formulae, that is, a Boolean combination of formulae of the shapes

$$\mathsf{Q}y\ \mathrm{sph}_\tau(y) \qquad \text{and} \qquad \mathrm{sph}_\varrho(\overline{x})$$

with $\mathsf{Q} \subseteq \mathbb{N}$ and σ-types τ and ϱ with one and ≥ 1 centres, respectively.

We also say that ψ is in *Hanf normal form*. The *locality radius* of ψ is the maximum of the locality radii of its counting-sentences and sphere-formulae.

Extending the proof of Proposition 3.1.6 it can be shown that for each degree bound $d \geq 0$, every $\mathsf{FO}[\sigma]$-formula is d-equivalent to a HNF-formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$.

In the following, we look beyond plain first-order logic and examine which extensions of first-order logic by unary counting quantifiers permit Hanf normal form. For this purpose, suppose that L is one of the logics defined in Section 2.4.2, that is, one of the logics $\mathsf{FO}{+}\mathrm{un}\mathsf{T}$, $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)$ with $D \subseteq D_{\mathrm{all}}$, or $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)$ with $C \subseteq C_{\mathrm{all}}$, or one of the corresponding tuple-counting logics $\mathsf{FO}{+}\mathrm{un}\mathsf{T}_{\mathrm{tpl}}$, $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}$, or $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)_{\mathrm{tpl}}$ defined in Section 2.4.2.

Definition 3.1.10. L *permits Hanf normal form* if for each degree bound $d \geq 0$, every relational signature σ, and every $\mathsf{L}[\sigma]$-formula $\varphi(\overline{x})$, there is a d-equivalent HNF-formula in $\mathsf{L}[\sigma]$.

In the course of this thesis, we will give a complete answer to the following two questions:

(1) Which logics L permit Hanf normal form?

(2) If a logic L permits Hanf normal form, (how) can L-formulae be turned effectively into HNF-formulae from L?

Towards the first question, we already know from Hanf's theorem that $\mathsf{FO}{+}\mathrm{un}\mathsf{T}$ permits Hanf normal form (recall that, according to Remark 3.1.8, threshold-counting quantifiers can be defined in plain first-order logic with a slight increase of quantifier rank and formula size). Furthermore, we know that these Hanf normal forms can, at least in the way they are defined in [BK12], be computed effectively.

For the extension of FO by a *single* modulo-counting quantifier D_p with period $p \geq 2$, Nurmonen's locality theorem [Nur00] extends Hanf's theorem by one additional condition, requesting that

(3) For every type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$, $|\tau(\mathcal{A})| \equiv |\tau(\mathcal{B})| \mod p$.

Extending the proof of Proposition 3.1.6, this leads to the observation that also $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(\{\mathsf{D}_p\})$ for a *single* modulo-counting quantifier D_p with $p \geq 2$ permits Hanf normal form.

In this chapter, we show that, for arbitrary $D \subseteq D_{\text{all}}$, the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)$ permits Hanf normal form. Moreover, we describe an effective procedure that leads to a worst-case optimal elementary algorithm to transform formulae over relational signatures from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)$ into d-equivalent HNF-formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)$, which takes 3-fold exponential time in the size of the input formula for degree bounds $d \geq 3$ and 2-fold exponential time for $d \leq 2$.

The remainder of this chapter points out two consequences of this result: In Section 3.3, we obtain an alternative proof of Nurmonen's locality theorem [Nur00] for $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$. We will later make use of this locality theorem in Chapter 6.

In Section 3.4, we use our algorithm for the construction of HNF-formulae for $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ to generalise Seese's model-checking algorithm for plain first-order logic [See96] on classes of structures of bounded degree to input formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$.

The algorithm for the construction of HNF-formulae for $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$, as well as the generalisation of Seese's model-checking algorithm were published in [HKS16], where both results were also extended to ultimately periodic quantifiers (see Chapter 8).

3.2 Modulo-Counting Quantifiers

In this section we show that for every degree bound $d \geq 2$, each formula φ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ over a relational signature has a d-equivalent HNF-formula ψ in $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ over the same signature and with the same modulo-counting quantifiers. Furthermore, we show that ψ can be computed effectively from φ.

The precise statement of this section's main result is as follows:

Theorem 3.2.1. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$,
- *a relational signature* σ, *and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ *with* $D \subseteq D_{\mathrm{all}}$,

computes a HNF*-formula* $\psi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ *that is* d*-equivalent to* $\varphi(\overline{x})$.

Let $T, P, n, q \geq 0$ *be the threshold, the maximum period, the number of free variables, and the quantifier rank of* $\varphi(\overline{x})$*, respectively. Then, the computed formula* $\psi(\overline{x})$ *has locality radius* $\leq 4^q$ *and threshold*

$$< \; T + (n{+}q) \cdot \nu_d(4^q).$$

Moreover, the algorithm constructs $\psi(\overline{x})$ *in time*

$$(2\max\{1, T, P\})^{(||\varphi|| \cdot \nu_d(4^q))^{\mathcal{O}(||\sigma||)}}.$$

Note that every HNF-formula that is d-equivalent to the input formula φ is also d'-equivalent to φ for each $d' < d$.

Remark 3.2.2. Clearly, $T, P, n, q < ||\varphi||$. Thus, under the assumption that σ contains only the relation symbols that actually occur in φ, that is, $||\sigma|| < ||\varphi||$, we can conclude that for every degree bound $d \geq 3$, the algorithm of Theorem 3.2.1 takes 3-fold exponential time

$$2^{d^{2^{\mathcal{O}(||\varphi||)}}}$$

in the size of φ, and the threshold of ψ is in $d^{2^{\mathcal{O}(||\varphi||)}}$.

Moreover, for degree bound $d = 2$, the algorithm takes 2-fold exponential time

$$2^{2^{\mathrm{poly}(||\varphi||)}}$$

and ψ has threshold in $2^{\mathcal{O}(||\varphi||)}$.

For the special case of input sentences from FO, Theorem 3.2.1 implies the algorithm for the construction of Hanf normal form from [BK12, HKS13].

The algorithm of Theorem 3.2.1 proceeds by induction over the shape of the input formula φ. In the base step, we transform quantifier-free formulae into Hanf normal form. In the inductive step, we have to handle formulae of the form $\neg\psi'$, $\psi' \vee \psi''$, and $(\mathsf{Q}{+}k)x_{n+1}\,\psi'(\overline{x}, x_{n+1})$ where ψ' and ψ'' already are HNF-formulae, and where Q is either $\exists$ or a modulo-counting quantifier. The first two cases of negations and disjunctions do not pose any problems since the set of HNF-formulae is closed under Boolean combinations.

The crucial step is to turn a formula $\varphi(\overline{x}) = (\mathsf{Q}{+}k)x_{n+1}\,\psi'(\overline{x}, x_{n+1})$, where the quantified formula $\psi'(\overline{x}, x_{n+1})$ is already a HNF-formula, into a d-equivalent HNF-formula. In the following Section 3.2.1, this is done in two steps: First, we construct a Boolean combination of counting-*formulae* that is d-equivalent to $\varphi(\overline{x})$. Then, we turn each counting-formula that is not already a counting-sentence into a d-equivalent HNF-formula.

In Section 3.2.2, the construction from Section 3.2.1 is employed in the inductive proof of Theorem 3.2.1.

In the following, we denote by σ a relational signature and by $d \geq 2$ a degree bound. A central observation, used throughout the steps of the proof is that there is only a finite number (which grows, in fact, 2-fold exponentially with r) of non-isomorphic d-bounded σ-types with radius r and n centres; and that the r-sphere of any tuple $\overline{a} \in A^n$ in an arbitrary d-bounded σ-structure $\mathcal{A}$ belongs to precisely one of these isomorphism classes.

In particular, this allows us to replace formulae by disjunctions of formulae which are only evaluated in interpretations where the r-sphere around the assignment of the free variables realises a certain fixed type. These formulae can then be simplified using knowledge about the shape of this type.

Recall that for all $d, r \geq 0$ and $n \geq 1$, we denote by $\mathfrak{T}_r^{d,\sigma}(n)$ a set of representatives of the isomorphism classes of all d-bounded σ-types with radius r and n centres. In particular, for each d-bounded σ-structure $\mathcal{A}$ and for every tuple $\overline{a} \in A^n$, there is exactly one $\tau \in \mathfrak{T}_r^{d,\sigma}(n)$ such that $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \tau$.

Consider two $\mathsf{L}[\sigma]$-formulae $\varphi(\overline{x})$ and $\psi(\overline{x})$ of some logic L (e.g., for this section, FO+unM). Suppose that $\overline{x}$ is a tuple of $n \geq 1$ pairwise distinct variables, and let τ be a σ-type with radius $r \geq 0$ and n centres. We call φ and ψ *equivalent with respect to* τ if in each σ-structure $\mathcal{A}$,

$$\mathcal{A} \models \varphi[\overline{a}] \quad \text{iff} \quad \mathcal{A} \models \psi[\overline{a}] \quad \text{for all } \overline{a} \in A^n \text{ with } \mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \tau.$$

The following observation will be used frequently during this section.

Observation 3.2.3. *Let $d, r \geq 0$, and let $n \geq 1$. Let $\varphi(\overline{x})$ be an $\mathsf{L}[\sigma]$-formula whose free variables are among the tuple $\overline{x}$ of length n. For each $\tau \in \mathfrak{T}_r^{d,\sigma}(n)$, suppose that $\varphi_\tau(\overline{x})$ is an $\mathsf{L}[\sigma]$-formula that is equivalent to $\varphi(\overline{x})$ with respect to τ. Then, $\varphi(\overline{x})$ is d-equivalent to the formula*

$$\bigvee_{\tau \in \mathfrak{T}_r^{d,\sigma}(n)} \Big(\mathrm{sph}_\tau(\overline{x}) \ \wedge \ \varphi_\tau(\overline{x}) \Big).$$

3.2.1 The Inductive Step for Quantifiers

This section describes how to turn formulae of the shape $(\mathsf{Q}{+}k)x_{n+1}\,\psi'(\overline{x}, x_{n+1})$, where the quantified formula $\psi'(\overline{x}, x_{n+1})$ is already a HNF-formula, again into a d-equivalent HNF-formula. This forms the crucial part of the inductive construction of HNF-formulae for arbitrary formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$. The transformation is summarised in Lemma 3.2.4.

The algorithm consists of two main parts: In a first step, the input formula is turned into a Boolean combination of counting-formulae. Here, the divide-and-conquer strategy of Section 2.9 leads to a sufficiently small Boolean combination. In a second step, Lemma 3.2.6 turns proper counting-formulae, that is, counting-formulae with free variables, into HNF-formulae.

Lemma 3.2.4. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *a relational signature σ, and*
- *a formula $\varphi(\overline{x}) = (\mathsf{Q}{+}k)x_{n+1}\,\psi'(\overline{x}, x_{n+1})$ from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$, where $D \subseteq D_{\mathrm{all}}$, $\mathsf{Q} \in D \cup \{\exists\}$, $k \geq 0$, $\overline{x}$ is a tuple of $n \geq 0$ free variables, and $\psi'(\overline{x}, x_{n+1})$ is a HNF-formula with threshold $T \geq 0$,*

computes a HNF-formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ that is d-equivalent to $\varphi(\overline{x})$.

If $r \geq 1$ is an upper bound on the locality radius of $\psi'(\overline{x}, x_{n+1})$, then $\psi(\overline{x})$ has locality radius $\leq 4r$. Furthermore, $\psi(\overline{x})$ has threshold at most

$$T \quad \text{if } \mathsf{Q} \in D, \text{ or } \quad \max\{T, k + n \cdot \nu_d(2r{+}1)\} \quad \text{if } \mathsf{Q} = \exists.$$

Moreover, the algorithm constructs $\psi(\overline{x})$ in time

$$||\psi'|| \cdot (2\max\{k,p\})^{((n+1)\cdot\nu_d(4r))^{\mathcal{O}(||\sigma||)}},$$

where $p \geq 1$ is the period of Q (recall that the existential quantifier has period 1).

For the following proofs, we denote by $\top^\sigma$ a *tautological* HNF-*sentence*

$$\top^\sigma \;:=\; \exists y\ \mathrm{sph}_\tau(y) \vee \neg\exists y\ \mathrm{sph}_\tau(y),$$

where τ is an arbitrary σ-type with radius 0 and one centre, and we let $\bot^\sigma$ denote the *unsatisfiable* HNF-*sentence* $\neg\top^\sigma$.

Proof of Lemma 3.2.4. Let $d \geq 2$ be a degree bound and let σ be a relational signature. Furthermore, let $D \subseteq D_{\mathrm{all}}$ and let $\varphi(\overline{x}) = (\mathsf{Q}{+}k)x_{n+1}\,\psi'(\overline{x}, x_{n+1})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ where $\mathsf{Q} \in D \cup \{\exists\}$, $k \geq 0$, and $\psi'(\overline{x}, x_{n+1})$ is a HNF-formula of locality radius at most $r \geq 1$ and with threshold $T \geq 0$. Let $p \geq 1$ be the period of Q. Recall that $p = 1$ if and only if Q is the existential quantifier. Furthermore, recall that $k \in [0, p)$ if otherwise Q is a modulo-counting quantifier from D with a period $p \geq 2$.

The algorithm proceeds as follows:

(Step 1) Compute the set $\mathfrak{T}^{d,\sigma}_r(n{+}1)$ of all d-bounded σ-types with radius r and $n + 1$ centres.

(Step 2) Recall that $\psi'(\overline{x}, x_{n+1})$ is a HNF-formula and therefore a Boolean combination of sphere-formulae with free variables among $\overline{x}, x_{n+1}$ and of counting-sentences. In particular, every sphere-formula in $\psi'(\overline{x}, x_{n+1})$ has locality radius $\leq r$ and thus, its validity in a σ-interpretation $(\mathcal{A}, \overline{a}, a_{n+1})$ only depends on the r-sphere of $\overline{a}, a_{n+1}$ in $\mathcal{A}$.

Claim 1. *For each $\tau \in \mathfrak{T}^{d,\sigma}_r(n{+}1)$, there is a* HNF*-sentence ψ'_τ that is equivalent to $\psi'(\overline{x}, x_{n+1})$ with respect to τ.*

Before we prove Claim 1, note that, by Observation 3.2.3, $\psi'(\overline{x}, x_{n+1})$ is d-equivalent to the formula

$$\bigvee_{\tau \in \mathfrak{T}^{d,\sigma}_r(n+1)} \Big(\mathrm{sph}_\tau(\overline{x}, x_{n+1}) \;\wedge\; \psi'_\tau \Big).$$

Proof of Claim 1. Let $\tau \in \mathfrak{T}^{d,\sigma}_r(n{+}1)$. Recall that τ is a σ-type with $n + 1$ centres, that is, a structure $(\mathcal{B}, \overline{b}, b_{n+1})$ over the signature $(\sigma, c_1, \ldots, c_n, c_{n+1})$. Consider a sphere-formula $\mathrm{sph}_\varrho(x_{i_1}, \ldots, x_{i_m})$ from $\psi'(\overline{x}, x_{n+1})$ with $m \in [1, n{+}1]$ free variables $(x_{i_1}, \ldots, x_{i_m})$ from $\overline{x}$, for suitable indices $1 \leq i_1 < \cdots < i_m \leq n + 1$. We check whether $\mathcal{B} \models \mathrm{sph}_\varrho[b_{i_1}, \ldots, b_{i_m}]$, that is, whether $\mathcal{N}^{\mathcal{B}}_s(b_{i_1}, \ldots, b_{i_m}) \cong \varrho$, where

$s \le r$ is the radius of ϱ, and replace $\mathrm{sph}_\varrho(x_{i_1}, \dots, x_{i_m})$ by

$$\begin{array}{ll} \top^\sigma & \text{if } \mathcal{N}_s^{\mathcal{B}}(b_{i_1}, \dots, b_{i_m}) \cong \varrho, \text{ or by} \\ \bot^\sigma & \text{if } \mathcal{N}_s^{\mathcal{B}}(b_{i_1}, \dots, b_{i_m}) \not\cong \varrho. \end{array}$$

This completes the proof of Claim 1.

(Step 3) From Step (2) we obtain that $\varphi(\overline{x})$ is d-equivalent to the formula

$$(\mathsf{Q}{+}k)x_{n+1} \bigvee_{\tau \in \mathfrak{T}_r^{d,\sigma}(n+1)} \Big(\mathrm{sph}_\tau(\overline{x}, x_{n+1}) \ \wedge \ \psi'_\tau \Big). \tag{1}$$

Observe that for each σ-structure $\mathcal{A}$ and each tuple $\overline{a} \in A^n$, the sets

$$\Big\{ \ a_{n+1} \in A \ : \quad (\mathcal{A}, \overline{a}, a_{n+1}) \ \models \ \mathrm{sph}_\tau(\overline{x}, x_{n+1}) \wedge \psi'_\tau \ \Big\}$$

for all types $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$ are pairwise disjoint, and let

$$\delta_\tau^i(\overline{x}) \ :\!= \quad (\mathsf{Q}{+}i)x_{n+1} \Big(\mathrm{sph}_\tau(\overline{x}, x_{n+1}) \ \wedge \ \psi'_\tau \Big)$$

for all $i \ge 0$ and $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$.

In the following, we describe how to replace Formula (1) by a sufficiently small equivalent Boolean combination of formulae $\delta_\tau^i(\overline{x})$ with $i \ge 0$ and $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$. To this aim, we make a case distinction on the shape of the quantifier $(\mathsf{Q}{+}k)$.

(Case 1) If $(\mathsf{Q}{+}k) = \exists^{\equiv k \bmod p}$ for $k \in [0, p)$, then Formula (1) is equivalent to the formula

$$\bigvee_{f \in F} \ \bigwedge_{\tau \in \mathfrak{T}_r^{d,\sigma}(n+1)} \delta_\tau^{f(\tau)}(\overline{x})$$

where F is the set of all functions $f\colon \mathfrak{T}_r^{d,\sigma}(n{+}1) \to [0, p)$ such that the sum of the values $f(\tau)$ for all $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$ is congruent to k modulo p. Unfortunately, this formula grows exponentially with the cardinality of the set $\mathfrak{T}_r^{d,\sigma}(n{+}1)$ and thus would lead to a 4-fold exponential size of the final constructed Hanf normal form in terms of the quantifier rank of the input formula.

However, by Lemma 2.9.2, we know that the latter formula is equivalent to the Boolean combination

$$\delta(\overline{x}) \ :\!= \quad \langle \delta_\tau^i \rangle^{\equiv k \bmod p}_{\mathfrak{T}_r^{d,\sigma}(n+1)}$$

of formulae $\delta_\tau^\ell(\overline{x})$ with $\ell \in [0, p)$ and $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$.

(Case 2) *If* $(\mathsf{Q}{+}k) = \exists^{>k}$, then Formula (1) is equivalent to the formula

$$\bigvee_{g \in G} \ \bigwedge_{\substack{\tau \in \mathfrak{T}_r^{d,\sigma}(n+1), \\ g(\tau) \geq 0}} \delta_\tau^{g(\tau)}(\overline{x})$$

where G is the set of all functions $g\colon \mathfrak{T}_r^{d,\sigma}(n{+}1) \to [-1, k]$ such that the values $g(\tau){+}1$ for all $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$ add up to $k+1$. By Lemma 2.9.4, we know that this formula is equivalent to the Boolean combination

$$\delta(\overline{x}) \ \coloneqq \ \langle \delta_\tau^i \rangle^{>k}_{\mathfrak{T}_r^{d,\sigma}(n+1)}$$

of formulae $\delta_\tau^\ell(\overline{x})$ with $\ell \in [0, k]$ and $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$.

(Step 4) Any formula $\delta_\tau^\ell(\overline{x})$ is of the shape

$$(\mathsf{Q}{+}\ell)x_{n+1} \left(\mathrm{sph}_\tau(\overline{x}, x_{n+1}) \ \wedge \ \psi'_\tau \right)$$

and thus equivalent to

$$\begin{aligned} \neg\psi'_\tau \ \vee \ (\mathsf{Q}{+}\ell)x_{n+1} \ \mathrm{sph}_\tau(\overline{x}, x_{n+1}) & \quad \text{if } (\mathsf{Q}{+}\ell) = \exists^{\equiv 0 \bmod p}, \text{ and to} \\ \psi'_\tau \ \wedge \ (\mathsf{Q}{+}\ell)x_{n+1} \ \mathrm{sph}_\tau(\overline{x}, x_{n+1}) & \quad \text{otherwise.} \end{aligned}$$

Carrying out these replacements in the formula $\delta(\overline{x})$ obtained in Step (3) we obtain a Boolean combination $\chi(\overline{x})$ of counting-formulae with locality radius $\leq r$.

In particular, if $n = 0$, that is, $\overline{x}$ is the empty tuple, then χ is a Boolean combination of counting-sentences and thus in Hanf normal form. In this case, the construction is complete and we let $\psi \coloneqq \chi$. Otherwise, we proceed with the next Step (5).

(Step 5) If $n \geq 1$, then $\chi(\overline{x})$ is a Boolean combination of

(a) counting-sentences with threshold $\leq T$ and locality radius $\leq r$, originating from the HNF-sentences ψ'_τ and thus from $\psi'(\overline{x}, x_{n+1})$, and

(b) counting-formulae of the shape $(\mathsf{Q}{+}\ell)x_{n+1}\,\mathrm{sph}_\tau(\overline{x}, x_{n+1})$ where either $(\mathsf{Q}{+}\ell) = \exists^{>\ell}$ for an $\ell \in [0, k]$ or $(\mathsf{Q}{+}\ell) = \exists^{\equiv \ell \bmod p}$ for an $\ell \in [0, p)$, and where τ is a type from the set $\mathfrak{T}_r^{d,\sigma}(n{+}1)$.

To obtain a HNF-formula $\psi(\overline{x})$ from $\chi(\overline{x})$, we employ Lemma 3.2.5, which is stated below. The lemma allows us to turn each counting-formula of

Shape (b) in $\chi(\overline{x})$ into a d-equivalent HNF-formula. By Lemma 3.2.5, all of the resulting HNF-formulae have locality radius $\leq 4r$ and thus, the same holds for the constructed HNF-formula $\psi(\overline{x})$.

This completes the construction of the HNF-formula $\psi(\overline{x})$. In the following, we complete the proof of Lemma 3.2.4 by an analysis of the threshold of $\psi(\overline{x})$ and by an analysis of the time required for its construction.

Threshold of $\psi(\overline{x})$. For a bound on the threshold of the constructed HNF-formula, recall that the formulae ψ'_τ for each $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$ have threshold $\leq T$.

(Case 1) *If* $(\mathsf{Q}{+}k) = \exists^{\equiv k \bmod p}$, the formulae $\delta(\overline{x}), \chi(\overline{x})$, and $\psi(\overline{x})$ also have threshold T, irrespective of the number of free variables.

(Case 2) *If* $(\mathsf{Q}{+}k) = \exists^{>k}$, the formula $\delta(\overline{x})$, obtained in Step (3), and thus, also the formula $\chi(\overline{x})$ from Step (4), have threshold $\max\{T, k\}$.

If $n = 0$, also $\psi = \chi$ has threshold $\max\{T, k\}$.

If $n \geq 1$, Step (5) applies Lemma 3.2.6, resulting in a HNF-formula $\psi(\overline{x})$ with threshold $\leq \max\{T, k + n \cdot \nu_d(2r{+}1)\}$.

We complete the proof of Lemma 3.2.4 by an analysis of the time required by the described algorithm to carry out Steps (1) to (5).

Time complexity. We number the steps of the computation in the same way as in the description of the algorithm and abbreviate the expression $(n{+}1) \cdot \nu_d(r)$ by N. Observe that $N \geq 2$, since $d \geq 2$ and $r \geq 1$.

(Step 1) According to Lemma 2.8.7, the set $\mathfrak{T}_r^{d,\sigma}(n{+}1)$ can be constructed in time

$$2^{N^{\mathcal{O}(||\sigma||)}}.$$

In particular, this implies that also $|\mathfrak{T}_r^{d,\sigma}(n{+}1)| \in 2^{N^{\mathcal{O}(||\sigma||)}}$.

(Step 2) The isomorphism test for an arbitrary type $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$ and a sphere-formula sph_ϱ from ψ' takes time in $2^{\mathcal{O}(||\sigma||)\cdot N^2}$, according to Lemma 2.8.6 (recall that ϱ has at most $n+1$ centres and locality radius $\leq r$).

Since $|\mathfrak{T}_r^{d,\sigma}(n{+}1)| \in 2^{N^{\mathcal{O}(||\sigma||)}}$ and ψ' contains at most $||\psi'||$ sphere-formulae, we obtain that the construction of the HNF-sentences ψ'_τ for all types $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$ takes time in

$$||\psi'|| \cdot 2^{N^{\mathcal{O}(||\sigma||)}} \cdot 2^{\mathcal{O}(||\sigma||)\cdot N^2} \quad \subseteq \quad ||\psi'|| \cdot 2^{N^{\mathcal{O}(||\sigma||)}}.$$

Clearly, each HNF-sentence ψ'_τ has size $\leq ||\psi'||$.

(Step 3) For the construction of the Boolean combination $\delta(\overline{x})$, recall from Lemma 2.8.8 that the formulae $\mathrm{sph}_\tau(\overline{x}, x_{n+1})$ for all $\tau \in \mathfrak{T}_r^{d,\sigma}(n{+}1)$ have size in $N^{\mathcal{O}(||\sigma||)}$ and can be constructed within the same time bound. Thus, each formula $\delta_\tau^i(\overline{x})$ has size in $||(\mathsf{Q}{+}i)|| + N^{\mathcal{O}(||\sigma||)} + ||\psi'||$.

We know that $|\mathfrak{T}_r^{d,\sigma}(n{+}1)| \in 2^{N^{\mathcal{O}(||\sigma||)}}$ and thus, the recursion depth of the constructions described in Section 2.9 is at most

$$\lceil \log |\mathfrak{T}_r^{d,\sigma}(n{+}1)| \rceil + 1 \in N^{\mathcal{O}(||\sigma||)}.$$

We distinguish between the following cases:

(Case 1) *If* $(\mathsf{Q}{+}k) = \exists^{\equiv k \bmod p}$, all formulae $\delta_\tau^i(\overline{x})$ that occur in $\delta(\overline{x})$ have $i < p$ and thus, size in $2p + N^{\mathcal{O}(||\sigma||)} + ||\psi'||$. By Lemma 2.9.2, we can conclude that $\delta(\overline{x})$ can be constructed in time

$$(2p)^{N^{\mathcal{O}(||\sigma||)}} \cdot (2p + N^{\mathcal{O}(||\sigma||)} + ||\psi'||) \quad \subseteq \quad ||\psi'|| \cdot (2p)^{N^{\mathcal{O}(||\sigma||)}}.$$

(Case 2) *If* $(\mathsf{Q}{+}k) = \exists^{>k}$, all formulae $\delta_\tau^i(\overline{x})$ that occur in $\delta(\overline{x})$ have $i \leq k$ and thus, size in $k + N^{\mathcal{O}(||\sigma||)} + ||\psi'||$. By Lemma 2.9.4, we can conclude that $\delta(\overline{x})$ can be constructed in time

$$(2k{+}2)^{N^{\mathcal{O}(||\sigma||)}} \cdot (k{+}N^{\mathcal{O}(||\sigma||)}{+}||\psi'||) \quad \subseteq \quad ||\psi'|| \cdot (2k{+}2)^{N^{\mathcal{O}(||\sigma||)}}.$$

In summary, we can conclude that the construction of $\delta(\overline{x})$ in any case takes time in

$$||\psi'|| \cdot (2\max\{k,p\})^{N^{\mathcal{O}(||\sigma||)}}$$

(Step 4) The construction of the formula $\chi(\overline{x})$ from $\delta(\overline{x})$ can be carried out in time $\mathcal{O}(||\delta||)$ and thus also takes time in $||\psi'|| \cdot (2\max\{k,p\})^{N^{\mathcal{O}(||\sigma||)}}$.

(Step 5) For each counting-formula of the shape $(\mathsf{Q}{+}\ell)x_{n+1}\ \mathrm{sph}_\tau(\overline{x}, x_{n+1})$ in $\chi(\overline{x})$, the algorithm from Lemma 3.2.5 requires time in

$$(2\max\{\ell,p\}) \cdot 2^{(n \cdot \nu_d(4r))^{\mathcal{O}(||\sigma||)}}.$$

Clearly, $\chi(\overline{x})$ contains at most $||\chi||$ such counting-formulae, and the size of χ is bounded by the time required for its construction. Furthermore, $\ell \leq k$. Thus, Step (5) can be performed in time

$$\begin{aligned} & ||\psi'|| \cdot (2\max\{k,p\})^{N^{\mathcal{O}(||\sigma||)}} \cdot (2\max\{k,p\}) \cdot 2^{(n\cdot\nu_d(4r))^{\mathcal{O}(||\sigma||)}} \\ \subseteq \quad & ||\psi'|| \cdot (2\max\{k,p\})^{((n+1)\cdot\nu_d(4r))^{\mathcal{O}(||\sigma||)}}. \end{aligned}$$

Summing up the time needed to perform Steps (1) to (5), we obtain that the described algorithm can be carried out in time

$$||\psi'|| \cdot (2\max\{k,p\})^{((n+1)\cdot\nu_d(4r))^{\mathcal{O}(||\sigma||)}}.$$

This completes the proof of Lemma 3.2.4. □

It remains to show how proper counting-formulae, that is, counting-formulae with free variables can be turned into d-equivalent HNF-formulae.

Lemma 3.2.5. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *a relational signature σ, and*
- *a counting-formula $\alpha(\overline{x}) := (\mathsf{Q}{+}\ell)x_{n+1}\ \mathrm{sph}_\tau(\overline{x}, x_{n+1})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$, where $\overline{x}$ is a tuple of $n \geq 1$ free variables and τ is a σ-type with $n+1$ centres and radius at most $r \geq 1$,*

computes a HNF*-formula $\beta(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$ that is d-equivalent to $\alpha(\overline{x})$.*

In particular, if $(\mathsf{Q}{+}\ell) = \exists^{\equiv \ell \bmod p}$ for a period $p \geq 2$, then $\beta(\overline{x})$ is a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(\{\mathsf{D}_p\})[\sigma]$ and of threshold 0. Otherwise, that is, if $(\mathsf{Q}{+}\ell) = \exists^{>\ell}$, then $\beta(\overline{x})$ is a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ and has threshold $\leq \ell + n \cdot \nu_d(2r{+}1)$.

Furthermore, the algorithm computes $\beta(\overline{x})$ in time

$$(2\max\{\ell,p\}) \cdot 2^{(n\cdot\nu_d(4r))^{\mathcal{O}(||\sigma||)}},$$

where $p \geq 1$ is the period of Q (recall that the existential quantifier has period 1).

For the proof of Lemma 3.2.5, which can be found further down below, we show a result about arbitrary unary counting quantifiers from which it is straightforward to derive the special case of modulo-counting and threshold-counting quantifiers required for the proof of Lemma 3.2.4. For the following, we generalise the threshold of formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ to formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(\{\mathsf{Q}\})$, where Q is an arbitrary unary counting quantifier: The *shift* of a formula φ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(\{\mathsf{Q}\})$ is the smallest $K \in \mathbb{N}$, such that φ only uses quantifiers $(\mathsf{Q}{+}k)$ with $k \leq K$.

Lemma 3.2.6. *Let $d \geq 2$ be a degree bound, let σ be a relational signature, and let*

$$\alpha(\overline{x}) \ := \ \mathsf{Q}x_{n+1}\ \mathrm{sph}_\tau(\overline{x}, x_{n+1})$$

be a counting-formula with $\mathsf{Q} \subseteq \mathbb{N}$*, a tuple* $\overline{x}$ *of* $n \geq 1$ *free variables, and a* σ*-type* τ *with* $n+1$ *centres and radius at most* $r \geq 1$*.*

There is a HNF*-formula* $\beta(\overline{x})$ *in* $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(\{\mathsf{Q}\})[\sigma]$ *that is* d*-equivalent to* $\alpha(\overline{x})$*. Moreover,* $\beta(\overline{x})$ *has locality radius* $\leq 4r$ *and shift* $\leq n \cdot \nu_d(2r{+}1)$*.*

Furthermore, for ultimately periodic Q*, there is an algorithm which computes* $\beta(\overline{x})$*, on input of* d*,* σ*, and* $\alpha(\overline{x})$*, in time*

$$||\mathsf{Q}|| \cdot 2^{(n \cdot \nu_d(4r))^{\mathcal{O}(||\sigma||)}}.$$

Proof. Let σ be a relational signature, and let $\alpha(\overline{x}) \coloneqq \mathsf{Q}x_{n+1}\ \mathrm{sph}_\tau(\overline{x}, x_{n+1})$ be a counting-formula where $\mathsf{Q} \subseteq \mathbb{N}$, $\overline{x} = (x_1, \dots, x_n)$ is a tuple of $n \geq 1$ free variables, and where τ is a σ-type with radius at most $r \geq 1$ and $n+1$ centres $\overline{c}, c_{n+1} = (c_1, \dots, c_n, c_{n+1})$.

The crucial combinatorial argument lies in the following claim.

Claim 1. *For every* $\varrho \in \mathfrak{T}^{d,\sigma}_{4r}(n)$ *there is a* HNF*-sentence* β_ϱ *in* $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(\{\mathsf{Q}\})[\sigma]$ *that is equivalent to* $\alpha(\overline{x})$ *with respect to* ϱ*, and that has locality radius* $\leq r$ *and shift* $\leq n \cdot \nu_d(2r{+}1)$*.*

Using Claim 1, it follows from Observation 3.2.3 that $\alpha(\overline{x})$ is d-equivalent to the HNF-formula

$$\beta(\overline{x}) \;\coloneqq\; \bigvee_{\varrho \in \mathfrak{T}^{d,\sigma}_{4r}(n)} \Big(\mathrm{sph}_\varrho(\overline{x}) \;\wedge\; \beta_\varrho \Big), \tag{1}$$

which also has shift $\leq n \cdot \nu_d(2r{+}1)$. The locality radius is determined by the sphere-formulae for the types from $\mathfrak{T}^{d,\sigma}_{4r}(n)$ and thus, $\beta(\overline{x})$ has locality radius $\leq 4r$.

Proof of Claim 1. Let $\varrho \in \mathfrak{T}^{d,\sigma}_{4r}(n)$ and let $\overline{b} = (b_1, \dots, b_n)$ denote the n centres of ϱ. The construction of the HNF-sentence β_ϱ proceeds by the following case distinction, which is also depicted in Figure 3.1.

(Case 1) If $c_{n+1} \in N^\tau_{2r+1}(\overline{c})$, then $N^\tau_r(\overline{c})$ intersects $N^\tau_r(c_{n+1})$ or some edge of the Gaifman graph of τ connects some element of the former set to some element of the latter set.

Hence, for each σ-structure $\mathcal{A}$ and every $\overline{a} \in A^n$, we have

$$\begin{aligned} & |\{a_{n+1} \in A \,:\, \mathcal{N}^{\mathcal{A}}_r(\overline{a}, a_{n+1}) \cong \tau\}| \\ = \quad & |\{a_{n+1} \in N^{\mathcal{A}}_{2r+1}(\overline{a}) \,:\, \mathcal{N}^{\mathcal{A}}_r(\overline{a}, a_{n+1}) \cong \tau\}|. \end{aligned} \tag{2}$$

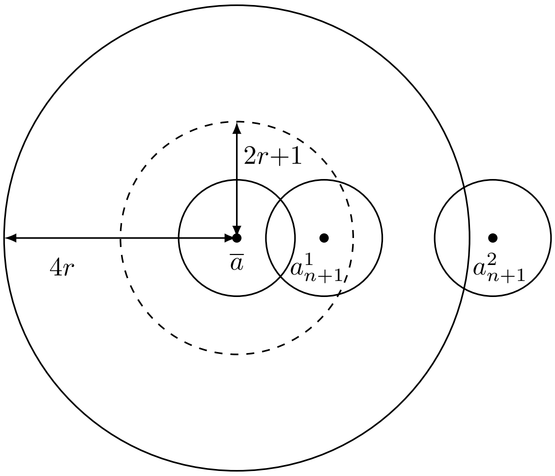

Figure 3.1 Case distinction in proof of Lemma 3.2.6. The nodes $a_{n+1}^{(1)}$ and $a_{n+1}^{(2)}$ depict witnesses for the quantifier Q in the formula $\alpha(\overline{x})$: For Case (1), that is, for the case $c_{n+1} \in N_{2r+1}^{\tau}(\overline{c})$, the node $a_{n+1}^{1} \in N_{2r+1}^{\mathcal{A}}(\overline{a})$ satisfies $\mathcal{N}_r^{\mathcal{A}}(\overline{a}, a_{n+1}^{1}) \cong \tau$, and for Case (2), that is, $c_{n+1} \notin N_{2r+1}^{\tau}(\overline{c})$, the node $a_{n+1}^{2} \in A \setminus N_{2r+1}^{\mathcal{A}}(\overline{a})$ satisfies $\mathcal{N}_r^{\mathcal{A}}(\overline{a}, a_{n+1}^{2}) \cong \tau$.

Since $(2r{+}1) + r = 3r + 1$, the set $N_r^{\tau}(c_{n+1})$ is a subset of the set $N_{3r+1}^{\tau}(\overline{c})$. Furthermore, since $3r + 1 \leq 4r$, we have

$$\begin{aligned} & |\{a_{n+1} \in N_{2r+1}^{\mathcal{A}}(\overline{a}) \,:\, \mathcal{N}_r^{\mathcal{A}}(\overline{a}, a_{n+1}) \cong \tau\}| \\ = \quad & |\{b_{n+1} \in N_{2r+1}^{\varrho}(\overline{b}) \,:\, \mathcal{N}_r^{\varrho}(\overline{b}, b_{n+1}) \cong \tau\}| \quad =: \ k_{\varrho}\,. \end{aligned} \tag{3}$$

for every σ-structure $\mathcal{A}$ and each tuple $\overline{a} \in A^n$ with $\mathcal{N}_{4r}^{\mathcal{A}}(\overline{a}) \cong \varrho$.

By Equation (2) and Equation (3), we can satisfy Claim 1 by choosing the HNF-sentence

$$\beta_{\varrho} \ := \ \begin{cases} \top^{\sigma} & \text{if } k_{\varrho} \in \mathsf{Q}, \quad \text{and} \\ \bot^{\sigma} & \text{otherwise.} \end{cases}$$

(Case 2) If $c_{n+1} \notin N_{2r+1}^{\tau}(\overline{c})$, then the sets $N_r^{\tau}(\overline{c})$ and $N_r^{\tau}(c_{n+1})$ are disjoint and there are no edges in the Gaifman graph of τ between the nodes from $N_r^{\tau}(\overline{c})$ and the nodes from $N_r^{\tau}(c_{n+1})$. We distinguish between the cases that $\mathcal{N}_r^{\tau} \ncong \mathcal{N}_r^{\varrho}(\overline{e})$ and that $\mathcal{N}_r^{\tau} \cong \mathcal{N}_r^{\varrho}(\overline{e})$:

(Case 2.a) If $\mathcal{N}_r^{\tau}(\overline{c})$ and $\mathcal{N}_r^{\varrho}(\overline{e})$ are not isomorphic, then, in each σ-structure $\mathcal{A}$ and for every tuple $\overline{a} \in A^n$ with $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \varrho$, the set of nodes $a_{n+1} \in A$ where $\mathcal{N}_r^{\mathcal{A}}(\overline{a}, a_{n+1}) \cong \tau$ is empty. Thus, Claim 1 can be satisfied by choosing the

HNF-sentence

$$\beta_\varrho \;:=\; \begin{cases} \top^\sigma & \text{if } 0 \in \mathsf{Q}, \quad \text{and} \\ \bot^\sigma & \text{otherwise.} \end{cases}$$

(Case 2.b) If $\mathcal{N}_r^\tau(\overline{c})$ and $\mathcal{N}_r^\varrho(\overline{e})$ are isomorphic, we have for each tuple $\overline{a} \in A^n$ in every σ-structure $\mathcal{A}$ that

$$\begin{aligned} & |\{a_{n+1} \in A \,:\, \mathcal{N}_r^{\mathcal{A}}(\overline{a}, a_{n+1}) \cong \tau\}| \\ = \;\; & |\{a_{n+1} \in A \setminus N_{2r+1}^{\mathcal{A}}(\overline{a}) \,:\, \mathcal{N}_r^{\mathcal{A}}(a_{n+1}) \cong \mathcal{N}_r^\tau(c_{n+1})\}|. \end{aligned} \tag{4}$$

Furthermore, since $(2r{+}1) + r = 3r + 1 \leq 4r$, we have

$$\begin{aligned} & |\{a_{n+1} \in N_{2r+1}^{\mathcal{A}}(\overline{a}) \,:\, \mathcal{N}_r^{\mathcal{A}}(a_{n+1}) \cong \mathcal{N}_r^\tau(c_{n+1})\}| \\ = \;\; & |\{b_{n+1} \in N_{2r+1}^{\varrho}(\overline{b}) \,:\, \mathcal{N}_r^{\varrho}(b_{n+1}) \cong \mathcal{N}_r^\tau(c_{n+1})\}| \;:=\; \ell_\varrho \end{aligned} \tag{5}$$

whenever $\mathcal{N}_{4r}^{\mathcal{A}}(\overline{a}) \cong \varrho$.

Thus, combining Equations (4) and (5), we obtain that for all σ-structures $\mathcal{A}$ and all $\overline{a} \in A^n$ with $\mathcal{N}_{4r}^{\mathcal{A}}(\overline{a}) \cong \varrho$,

$$\begin{aligned} & |\{a_{n+1} \in A \,:\, \mathcal{N}_r^{\mathcal{A}}(\overline{a}, a_{n+1}) \cong \tau\}| \\ = \;\; & |\{a_{n+1} \in A \,:\, \mathcal{N}_r^{\mathcal{A}}(a_{n+1}) \cong \mathcal{N}_r^\tau(c_{n+1})\}| \;-\; \ell_\varrho. \end{aligned}$$

Hence, we can satisfy Claim 1 by choosing the HNF-sentence

$$\beta_\varrho \;:=\; (\mathsf{Q}{+}\ell_\varrho)y \; \mathrm{sph}_{\mathcal{N}_r^\tau(c_{n+1})}(y).$$

Clearly, the size of ℓ_ϱ is bounded by the number of elements that may exist in a d-bounded type with radius $2r + 1$ and n centres, and thus, β_ϱ has shift $\leq n \cdot \nu_d(2r{+}1)$.

Note that, in all cases of the construction, the HNF-sentence β_ϱ has locality radius $\leq r$ and shift $\leq n \cdot \nu_d(2r{+}1)$. This completes the proof of Claim 1.

For ultimately periodic Q, it can easily be decided for a number $m \in \mathbb{N}$ if $m \in \mathsf{Q}$. In Case (1) and Case (2.a) in the proof of Claim 1, this is used for $m = k_\varrho$ and $m = 0$, respectively, and leads to an algorithm which constructs the HNF-formula $\beta(\overline{x})$. We complete the proof of Lemma 3.2.6 by an analysis of the time complexity of this algorithm.

Time complexity. In the following, we abbreviate $N := n \cdot \nu_d(4r)$. Observe that $N \geq 2$, since $d \geq 2$ and $n, r \geq 1$.

By Lemma 2.8.7, the set $\mathfrak{T}_{4r}^{d,\sigma}(n)$ can be constructed in time

$$2^{N^{\mathcal{O}(||\sigma||)}}. \tag{6}$$

To obtain the HNF-formula $\beta(\overline{x})$, we have to construct the sphere-formula $\mathrm{sph}_\varrho(\overline{x})$ and the HNF-sentence β_ϱ for each type $\varrho \in \mathfrak{T}_{4r}^{d,\sigma}(n)$.

Let $\varrho \in \mathfrak{T}_{4r}^{d,\sigma}(n)$. By Lemma 2.8.8 it takes time

$$N^{\mathcal{O}(||\sigma||)} \tag{7}$$

to construct $\mathrm{sph}_\varrho(\overline{x})$. For the construction of β_ϱ according to Claim 1, we have to make a case distinction depending on whether $c_{n+1} \in N_{2r+1}^{\tau}(\overline{c})$.

To determine which of the two cases actually applies for the given type τ, recall that the universe of τ has size at most $(n+1) \cdot \nu_d(r)$. Thus, the time needed to decide whether $c_{n+1} \in N_{2r+1}^{\tau}(\overline{c})$ is in

$$N^{\mathcal{O}(||\sigma||)}. \tag{8}$$

(Case 1) If $c_{n+1} \in N_{2r+1}^{\tau}(\overline{c})$, we compute the number k_ϱ defined in Equation (3). This requires us to check for at most $n \cdot \nu_d(2r+1) \leq N$ types with radius r and $n+1$ centres whether they are isomorphic to τ. As each of these types is d-bounded, the number k_ϱ can be computed in time

$$N \cdot 2^{\mathcal{O}(||\sigma||) \cdot N^2} \quad \subseteq \quad 2^{\mathcal{O}(||\sigma||) \cdot N^2}$$

by using the brute-force isomorphism test described in the proof of Lemma 2.8.6.

The representation $\mathrm{rep}(\mathsf{Q})$ of the quantifier Q can be used for testing whether $k_\varrho \in \mathsf{Q}$. This takes time in $\mathcal{O}(k_\varrho)$. Since $k_\varrho \leq N$, the algorithm altogether constructs β_ϱ in Case (1) in time

$$2^{\mathcal{O}(||\sigma||) \cdot N^2} \tag{9}$$

(Case 2) *If* $c_{n+1} \notin N_{2r+1}^{\tau}(\overline{c})$, we have to check whether the two types $\mathcal{N}_r^{\tau}(\overline{c})$ and $\mathcal{N}_r^{\varrho}(\overline{b})$ are isomorphic. According to Lemma 2.8.6 this takes time in

$$2^{\mathcal{O}(||\sigma||) \cdot N^2}. \tag{10}$$

(Case 2.a) If $\mathcal{N}_r^{\tau}(\overline{c})$ and $\mathcal{N}_r^{\varrho}(\overline{b})$ are not isomorphic, we need constant time to check whether $0 \in \mathsf{Q}$ and to construct β_ϱ accordingly.

(Case 2.b) Otherwise, that is, if $\mathcal{N}_r^{\tau}(\bar{c})$ and $\mathcal{N}_r^{\varrho}(\bar{b})$ are isomorphic, we have to compute the number ℓ_ϱ defined in Equation (5) of the proof of Lemma 3.2.6. This requires us to check for at most $n \cdot \nu_d(2r{+}1) \leq N$ d-bounded types with radius r and one centre whether they are isomorphic to the type $\mathcal{N}_r^{\tau}(c_{n+1})$. By using the isomorphism test from Lemma 2.8.6, the number ℓ_ϱ can be computed in time

$$2^{\mathcal{O}(||\sigma||)\cdot N^2}.$$

Afterwards, we construct the counting-sentence β_ϱ. According to Lemma 2.8.8, we need time $N^{\mathcal{O}(||\sigma||)}$ to construct the formula $\mathrm{sph}_{\mathcal{N}_r^{\tau}(c_{n+1})}(y)$. Since, furthermore, $\ell_\varrho \leq N$, the counting-sentence β_ϱ can be constructed in time

$$\mathcal{O}(||(\mathsf{Q}{+}N)||) + N^{\mathcal{O}(||\sigma||)} \quad \subseteq \quad ||\mathsf{Q}|| \cdot N^{\mathcal{O}(||\sigma||)}. \tag{11}$$

We thus obtain from Estimate (10) and Estimate (11) that the algorithm uses altogether time in

$$2^{\mathcal{O}(||\sigma||)\cdot N^2} + ||\mathsf{Q}|| \cdot N^{\mathcal{O}(||\sigma||)} \quad \subseteq \quad ||\mathsf{Q}|| \cdot 2^{N^{\mathcal{O}(||\sigma||)}}. \tag{12}$$

to construct the formula β_ϱ of Case (2).

Finally, the algorithm outputs the HNF-formula $\beta(\overline{x})$, which is the disjunction of the formulae $(\mathrm{sph}_\varrho(\overline{x}) \wedge \beta_\varrho)$ for all $\varrho \in \mathfrak{T}_{4r}^{d,\sigma}(n)$. Using Estimates (6) to (9) and Estimate (12), the overall time required by the algorithm is in

$$2^{N^{\mathcal{O}(||\sigma||)}} + 2^{N^{\mathcal{O}(||\sigma||)}} \cdot \left(N^{\mathcal{O}(||\sigma||} + 2^{\mathcal{O}(||\sigma||)\cdot N^2} + ||\mathsf{Q}|| \cdot 2^{N^{\mathcal{O}(||\sigma||)}}\right)$$
$$\subseteq \quad ||\mathsf{Q}|| \cdot 2^{N^{\mathcal{O}(||\sigma||)}}.$$

This completes the proof of Lemma 3.2.6. $\square$

Proof of Lemma 3.2.5 using Lemma 3.2.6. Let $d \geq 2$ be a degree bound, let σ be a relational signature, let $\mathsf{D}_p \in D_{\mathrm{all}}$, and let $\alpha(\overline{x}) \coloneqq (\mathsf{Q}{+}\ell)x_{n+1}\ \mathrm{sph}_\tau(\overline{x}, x_{n+1})$ be a counting-formula from $\mathsf{FO}{+}\mathrm{unM}(\{\mathsf{D}_p\})[\sigma]$ with a tuple of $n \geq 1$ free variables, and a σ-type τ with radius at most $r \geq 1$ and $n+1$ centres. In particular, Q is either the modulo-counting quantifier D_p or the existential quantifier with period $p \coloneqq 1$.

Let $\beta'(\overline{x})$ be the HNF-formula from $\mathsf{FO}{+}\mathrm{unC}(\{(\mathsf{Q}{+}\ell)\})[\sigma]$, which the algorithm of Lemma 3.2.6 computes on input of d, σ, and $\alpha(\overline{x})$. Recall that $\beta'(\overline{x})$ has shift $\leq n \cdot \nu_d(2r{+}1)$.

(Case 1) *If* $\mathsf{Q} = \exists$, then $\beta'(\overline{x})$ is, in particular, a HNF-formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ with threshold $\leq \ell + n \cdot \nu_d(2r{+}1)$. Thus, we can choose $\beta(\overline{x}) \coloneqq \beta'(\overline{x})$.

(Case 2) *If* $\mathsf{Q} = \mathsf{D}_p$, then $\ell \in [0,p)$ and $\beta'(\overline{x})$ is a HNF-formula from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(\{(\mathsf{D}_p{+}\ell)\})[\sigma]$. We replace every counting-sentence of the shape $(\mathsf{D}_p{+}k)y\ \mathrm{sph}_\varrho(y)$ and with $k \geq p$ in $\beta'(\overline{x})$ by the counting-sentence $(\mathsf{D}_p{+}k')y\ \mathrm{sph}_\varrho(y)$, for which $k' \in [0,p)$ is chosen such that $k \equiv k' \mod p$. Afterwards, we output the resulting HNF-formula $\beta(\overline{x})$, which, in particular, belongs to $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(\{\mathsf{D}_p\})[\sigma]$.

Furthermore, $\beta(\overline{x})$ has threshold 0, since already $\beta'(\overline{x})$ only uses counting-sentences $(\exists{+}k)y\ \mathrm{sph}_\varrho(y)$ with $k = 0$.

Time complexity. Recalling the encoding of ultimately periodic quantifiers, we know that $||(\mathsf{Q}{+}\ell)|| \leq \max\{3{+}\ell, 2p\} \leq 2\max\{\ell,p\} + 3$. Thus, the construction of $\beta'(\overline{x})$ from $\alpha(\overline{x})$ takes time in

$$(2\max\{\ell,p\}) \cdot 2^{(n \cdot \nu_d(4r))^{\mathcal{O}(||\sigma||)}}. \tag{1}$$

As the construction of $\beta(\overline{x})$ from $\beta'(\overline{x})$ takes time linear in the size of $\beta'(\overline{x})$, Estimate (1) is also an upper bound on the time required to construct $\beta(\overline{x})$ from $\alpha(\overline{x})$. This completes the proof of Lemma 3.2.5. □

3.2.2 The Hanf Normal Form Algorithm

We are now ready to prove Theorem 3.2.1 – the main result of this chapter. The proof uses the induction step described in Section 3.2.1 to turn arbitrary formulae with modulo-counting quantifiers into Hanf normal form.

Proof of Theorem 3.2.1. We describe the algorithm on input of a degree bound $d \geq 2$, a relational signature σ, and a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$, where $D \subseteq D_{\mathrm{all}}$. Let $n \coloneqq |\overline{x}|$ be the number of free variables of φ and let $T, P, q \geq 0$ be the threshold, the maximum period, and the quantifier rank of φ, respectively.

The algorithm proceeds by induction on the shape of $\varphi(\overline{x})$. We will show that the following inductive invariant holds for the constructed HNF-formula $\psi(\overline{x})$:

Claim 1.

(a) $\psi(\overline{x})$ *is d-equivalent to* $\varphi(\overline{x})$.

(b) $\psi(\overline{x})$ *has locality radius* $\leq 4^q$.

(c) $\psi(\overline{x})$ *has threshold* $\leq T + (n{+}q) \cdot \nu_d(4^q)$.

(d) There is a number $c \in \mathbb{N}_{\geq 1}$ of size $\mathcal{O}(||\sigma||)$, such that the algorithm terminates after at most

$$(2 \max\{1, T, P\})^{(||\varphi|| \cdot \nu_d(4^q))^c}$$

time steps.

Suppose that $\varphi(\overline{x})$ is quantifier-free, that is, $q = 0$. Any type $(\mathcal{A}, \overline{a})$ from $\mathfrak{T}_0^{d,\sigma}(n)$ is described by the set of atomic formulae which hold for its centres $\overline{a}$. Hence, $\varphi(\overline{x})$ is d-equivalent to a disjunction of sphere-formulae for all the types from $\mathfrak{T}_0^{d,\sigma}(n)$ that satisfy $\varphi(\overline{x})$. In detail, we construct $\psi(\overline{x})$ as follows:

(Step 1) We let $\mathfrak{T} \subseteq \mathfrak{T}_0^{d,\sigma}(n)$ be the set that contains precisely those types $(\mathcal{A}, \overline{a})$ from $\mathfrak{T}_0^{d,\sigma}(n)$ for which $\mathcal{A} \models \varphi[\overline{a}]$.

(Step 2) If $\mathfrak{T}$ is the empty set, there is no d-bounded σ-structure $\mathcal{A}$ with a tuple $\overline{a} \in A^n$ for which $\mathcal{A} \models \varphi[\overline{a}]$. Hence, $\varphi(\overline{x})$ is d-equivalent to the unsatisfiable HNF-formula

$$\psi(\overline{x}) \quad := \quad \mathrm{sph}_\tau(\overline{x}) \ \wedge \ \neg\, \mathrm{sph}_\tau(\overline{x}),$$

where τ is an arbitrary type from $\mathfrak{T}_0^{d,\sigma}(n)$. Otherwise, we let

$$\psi(\overline{x}) \quad := \quad \bigvee_{\tau \in \mathfrak{T}} \mathrm{sph}_\tau(\overline{x}).$$

In both cases, $\psi(\overline{x})$ is a HNF-formula with locality radius 0 and threshold 0. Hence, Statements (a) to (c) of Claim 1 are satisfied.

The case of $\varphi(\overline{x})$ being a Boolean combination of formulae with quantifier rank $q \geq 1$ is straightforward: If $\varphi = \neg\varphi'$, we compute a HNF-formula ψ' that is d-equivalent to φ' and let $\psi := \neg\psi'$. If $\varphi = (\varphi' \vee \varphi'')$, we compute HNF-formulae ψ' and ψ'' that are d-equivalent to φ' and φ'', respectively, and let $\psi := (\psi' \vee \psi'')$. In both cases, the inductive invariant of Claim 1 is obviously satisfied.

In the case of a quantified formula $\varphi(\overline{x})$, that is,

$$\varphi(\overline{x}) \quad = \quad (\mathsf{Q}{+}k) x_{n+1}\, \varphi'(\overline{x}, x_{n+1})$$

with $(\mathsf{Q}{+}k) = \exists^{\equiv k \bmod p}$ for some $p \in [1, P]$ and $k \in [0, p)$ or $(\mathsf{Q}{+}k) = \exists^{>k}$ for a $k \in [0, T]$, and a formula $\varphi'(\overline{x}, x_{n+1})$ with quantifier rank $q - 1$, the algorithm proceeds along the following steps:

(Step 3) We call the algorithm recursively to compute a HNF-formula $\psi'(\overline{x}, x_{n+1})$ for which, according to the inductive invariant of Claim 1, the following holds:

(a') $\psi'(\overline{x}, x_{n+1})$ is d-equivalent to $\varphi'(\overline{x}, x_{n+1})$.

(b') $\psi'(\overline{x}, x_{n+1})$ has locality radius $\leq 4^{q-1}$.

(c') $\psi'(\overline{x}, x_{n+1})$ has threshold

$$\begin{aligned} T' &< T + ((n{+}1) + (q{-}1)) \cdot \nu_d(4^{q-1}) \\ &= T + (n{+}q) \cdot \nu_d(4^{q-1}). \end{aligned}$$

(Step 4) By using the algorithm of Lemma 3.2.4, we construct a HNF-formula $\psi(\overline{x})$ that is d-equivalent to the formula $(\mathsf{Q}{+}k)x_{n+1}\, \psi'(\overline{x}, x_{n+1})$. From Lemma 3.2.4 we know that $\psi(\overline{x})$ has locality radius $\leq 4 \cdot 4^{q-1} = 4^q$.

Furthermore, if $\mathsf{Q} \in D$, then $\psi(\overline{x})$ has threshold

$$T' \;<\; T + (n{+}q) \cdot \nu_d(4^{q-1}) \;<\; T + (n{+}q) \cdot \nu_d(4^q)$$

and, if $\mathsf{Q} = \exists$, then $\psi(\overline{x})$ has threshold

$$\begin{aligned} & \max\{T',\ k + n \cdot \nu_d(2 \cdot 4^{q-1} + 1)\} \\ \leq\ & \max\{T',\ T + n \cdot \nu_d(2 \cdot 4^{q-1} + 1)\} \\ =\ & \max\{T + (n{+}q) \cdot \nu_d(4^{q-1}),\ T + n \cdot \nu_d(2 \cdot 4^{q-1} + 1)\} \\ =\ & T + \max\{(n{+}q) \cdot \nu_d(4^{q-1}),\ n \cdot \nu_d(2 \cdot 4^{q-1} + 1)\} \\ <\ & T + (n{+}q) \cdot \nu_d(4^q). \end{aligned}$$

The latter inequality holds, since $2{\cdot}4^{q-1}{+}1 < 4^q$. Thus, the HNF-formula $\psi(\overline{x})$ satisfies Statements (a) to (c) of Claim 1.

Time complexity. For the analysis of the time complexity of the inductive construction, that is, for the proof of Statement (d) of Claim 1, we abbreviate $N := ||\varphi|| \cdot \nu_d(4^q)$ and let $B := 2\max\{1, T, P\}$. Conditions on a suitable choice of the number $c \in \mathbb{N}_{\geq 1}$ will be given during the course of the analysis.

The steps of the analysis are enumerated in the same way as the steps in the construction of ψ described above.

For the case of $\varphi(\overline{x})$ being quantifier-free, we estimate the time required to perform the following steps:

(Step 1) As $n < ||\varphi||$ and $\nu_d(0) = 1$, we know from Lemma 2.8.7 that the set $\mathfrak{T}_0^{d,\sigma}(n)$ can be computed in time $2^{||\varphi||^{\mathcal{O}(||\sigma||)}}$.

Since $\varphi(\overline{x})$ is quantifier-free, it only needs time $||\varphi||^{\mathcal{O}(||\sigma||)}$ to decide whether $\mathcal{A} \models \varphi[a_1, \ldots, a_n]$ for each type $(\mathcal{A}, a_1, \ldots, a_n) \in \mathfrak{T}_0^{d,\sigma}(n)$. Thus, the set $\mathfrak{T}$ can be computed in time

$$||\varphi||^{\mathcal{O}(||\sigma||)} \cdot 2^{||\varphi||^{\mathcal{O}(||\sigma||)}} \quad \subseteq \quad 2^{||\varphi||^{\mathcal{O}(||\sigma||)}}.$$

(Step 2) For each type $\tau \in \mathfrak{T}$, the sphere-formula $\mathrm{sph}_\tau(\overline{x})$ can be computed in time $||\varphi||^{\mathcal{O}(||\sigma||)}$, according to Lemma 2.8.8. Hence, the whole formula $\psi(\overline{x})$ can be computed in time

$$||\varphi||^{\mathcal{O}(||\sigma||)} \cdot 2^{||\varphi||^{\mathcal{O}(||\sigma||)}} \quad \subseteq \quad 2^{||\varphi||^{\mathcal{O}(||\sigma||)}}.$$

By adding up the time required for both steps, we can conclude that $c \in \mathbb{N}_{\geq 1}$ can be chosen of size $\mathcal{O}(||\sigma||)$ such that the algorithm terminates in at most

$$2^{||\varphi||^c} \quad \leq \quad B^{N^c}$$

time steps and thus, Statement (d) of Claim 1 is satisfied.

For $\varphi(\overline{x})$ being a Boolean combination of formulae with quantifier rank $q \geq 1$, Statement (d) of Claim 1 holds trivially.

Suppose that $\varphi(\overline{x})$ is a quantified formula of the shape $(\mathsf{Q}{+}k)x_{n+1}\,\varphi'(\overline{x}, x_{n+1})$, where Q has period $p \geq 1$. Again, we analyse the time required for the steps in the construction of $\psi(\overline{x})$.

(Step 3) According to Statement (d) of Claim 1, the algorithm constructs $\psi'(\overline{x}, x_{n+1})$ from $\varphi'(\overline{x}, x_{n+1})$ in at most

$$(2\max\{1, K, P\})^{(||\varphi'||\cdot\nu_d(4^{q-1}))^c} \quad \leq \quad B^{(N-1)^c}$$

time steps; and this is also an upper bound on the size of $\psi'(\overline{x}, x_{n+1})$.

(Step 4) By Lemma 3.2.4, the HNF-formula $\psi(\overline{x})$ can be computed from the formula $(\mathsf{Q}{+}k)x_{n+1}\,\psi'(\overline{x}, x_{n+1})$ in time

$$||\psi'|| \cdot (2\max\{k, p\})^{((n+1)\cdot\nu_d(4r))^{\mathcal{O}(||\sigma||)}}.$$

Since $2\max\{k, p\} \leq B$ and $(n{+}1) \cdot \nu_d(4r) \leq N$, there is a number $c' \in \mathbb{N}_{\geq 1}$ of size $\mathcal{O}(||\sigma||)$, such that the algorithm from Lemma 3.2.4 takes at most

$$B^{(N-1)^c} \cdot B^{N^{c'}} \quad = \quad B^{(N-1)^c + N^{c'}}$$

time steps.

Summing up the time needed for Step (3) and Step (4), the algorithm needs at most

$$B^{(N-1)^c} + B^{(N-1)^c + N^{c'}} \quad \leq \quad B^{(N-1)^c + N^{c''}}$$

time steps, where $c'' > c'$ is of size $\mathcal{O}(||\sigma||)$. Choosing $c := c'' + 1$, we obtain that

$$\begin{array}{rlcl} & (N-1)^c + N^{c''} & \leq & (N-1)^c + N^{c-1} \\ = & N^c \cdot \left(\left(\frac{N-1}{N}\right)^c + \frac{1}{N}\right) & \leq & N^c \cdot \left(\frac{N-1}{N} + \frac{1}{N}\right) \\ = & N^c. & & \end{array}$$

Thus, the algorithm requires at most

$$(2\max\{1, T, P\})^{(||\varphi||\cdot\nu_d(4^q))^c}$$

to construct $\psi(\overline{x})$. This shows that Statement (d) of Claim 1 is satisfied and concludes the proof of Theorem 3.2.1 $\square$

3.3 An Alternative Proof of Nurmonen's Locality Theorem

Hanf's [Han65, FSV95, EF99] and Nurmonen's [Nur00] locality theorems (cf. Section 3.1) lead to Hanf normal forms for the logics FO+unT and FO+unM$(\{\mathsf{D}_p\})$ for each $p \geq 2$. In this section, we take the other direction. More precisely, we use the construction of Hanf normal form for FO+unM, described in Theorem 3.2.1 in the previous section, to obtain an alternative and slightly generalised proof of Nurmonen's locality theorem that can be stated as follows:

Theorem 3.3.1. *Let σ be a relational signature and let $d \geq 2$ be a degree bound. Furthermore, let $T, n, q \geq 0$ and $M \geq 1$.*

Suppose that $\mathcal{A}$ and $\mathcal{B}$ are d-bounded σ-structures and that $\overline{a} \in A^n$ and $\overline{b} \in B^n$, such that the following Conditions (1) to (3) are satisfied for $r := 4^q$:

(1) $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \;\cong\; \mathcal{N}_r^{\mathcal{B}}(\overline{b})$.

For every type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$,

(2) $|\tau(\mathcal{A})| \;\equiv\; |\tau(\mathcal{B})| \mod M$, *and*

(3) either $|\tau(\mathcal{A})| \;=\; |\tau(\mathcal{B})|$ *or*

$$|\tau(\mathcal{A})|, |\tau(\mathcal{B})| \;\geq\; T + (n+q)\cdot\nu_d(r).$$

Then, for each tuple $\overline{x}$ of n distinct variables and every formula $\varphi(\overline{x})$ from FO+unM$[\sigma]$ *with threshold $\leq T$, quantifier rank $\leq q$, and such that M is a common multiple of the periods of all quantifiers that occur in $\varphi(\overline{x})$,*

$$\mathcal{A} \models \varphi[\overline{a}] \quad \textit{iff} \quad \mathcal{B} \models \varphi[\overline{b}].$$

For the special case of sentences from FO, Theorem 3.3.1 implies Hanf's Theorem as stated in, e.g., Theorem 2.4.1 of [EF99]. More generally, for sentences with threshold 0 from $\mathsf{FO}{+}\mathrm{unM}(\{\mathsf{D}_p\})$, for some period $p \geq 2$, Theorem 3.3.1 implies Nurmonen's theorem (Theorem 3.4 in [Nur00]). In fact, the game theoretical condition for elementary equivalence with respect to first-order logic with a modulo-counting quantifier, defined in [Nur00], and the subsequent combinatorial proof of Nurmonen's theorem there, can be extended to an alternative proof of Theorem 3.3.1.

Note that, due to the specific construction of Hanf normal form applied in the proof of Theorem 3.3.1 below, the locality radius $r := 4^q$ obtained in Theorem 3.3.1 grows faster with the quantifier rank as in Hanf's and Nurmonen's theorems, whose combinatorial proofs lead to locality radius 3^q.

Proof of Theorem 3.3.1. Let σ be a relational signature and let $d \geq 2$ be a degree bound. Furthermore, let $T, n, q \geq 0$, $M \geq 1$, and let $r := 4^q$.

Suppose that $\mathcal{A}$ and $\mathcal{B}$ are d-bounded σ-structures and that furthermore $\overline{a} = (a_1, \dots, a_n) \in A^n$ and $\overline{b} = (b_1, \dots, b_n) \in B^n$, such that Conditions (1) to (3) of Theorem 3.3.1 are satisfied.

Let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{unM}[\sigma]$. Let $D \subseteq D_{\text{all}}$ be the set of all modulo-counting quantifiers that appear in φ, and suppose that φ has threshold $\leq T$, quantifier rank $\leq q$, at most n free variables from a tuple $\overline{x} = (x_1, \dots, x_n)$, and that M is a common multiple of the periods of the quantifiers occurring in φ.

We want to show that

$$\mathcal{A} \models \varphi[\overline{a}] \quad \text{iff} \quad \mathcal{B} \models \varphi[\overline{b}]. \tag{1}$$

Let $\psi(\overline{x})$ the HNF-formula from $\mathsf{FO}{+}\mathrm{unM}(D)[\sigma]$, computed by Theorem 3.2.1 on input of d, σ, and $\varphi(\overline{x})$. In particular, $\psi(\overline{x})$ is d-equivalent to $\varphi(\overline{x})$ and, moreover, a Boolean combination of

(a) sphere-formulas $\mathrm{sph}_\varrho(\overline{x})$, where ϱ is a σ-type with radius $\leq r$ and at most n centres,

(b) counting-sentences $\exists^{>k} y\ \mathrm{sph}_\tau(y)$, where

$$k \ < \ T + (n{+}q) \cdot \nu_d(r)$$

and τ is a σ-type with radius $\leq r$ and one centre, and *(c)* counting-sentences $\exists^{\equiv k \bmod p} y\ \mathrm{sph}_\tau(y)$ where $p \geq 2$ divides M, $k \in [0, p)$, and τ is a σ-type with radius $\leq r$ and one centre.

Since $\varphi(\overline{x})$ and $\psi(\overline{x})$ are d-equivalent and $\mathcal{A}$, $\mathcal{B}$ are d-bounded, Equivalence (1) follows directly from the following claim.

Claim 1.

$$\mathcal{A} \models \psi[\overline{a}] \quad \textit{iff} \quad \mathcal{B} \models \psi[\overline{b}].$$

Proof of Claim 1 We show that for each subformula $\gamma(\overline{x})$ of $\psi(\overline{x})$ of Shape (a), Shape (b), or Shape (c),

$$\mathcal{A} \models \gamma[\overline{a}] \quad \text{iff} \quad \mathcal{B} \models \gamma[\overline{b}].$$

(a) Consider a sphere-formula $\mathrm{sph}_\varrho(x_{i_1}, \ldots, x_{i_m})$ from $\psi(\overline{x})$, where $x_{i_1}, \ldots, x_{i_m}$ are $m \in [1, n]$ pairwise distinct variables from $x_1, \ldots, x_n$ for suitable indices $i_1, \ldots, i_m \in [1, n]$, and where ϱ is a σ-type of radius $s \leq r$ and with m centres. The following equivalences hold:

$$\begin{array}{ll} & \mathcal{A} \models \mathrm{sph}_\varrho[a_{i_1}, \ldots, a_{i_m}] \\ \text{iff} & \mathcal{N}_s^{\mathcal{A}}(a_{i_1}, \ldots, a_{i_m}) \cong \varrho \\ \text{iff} & \mathcal{N}_s^{\mathcal{B}}(b_{i_1}, \ldots, b_{i_m}) \cong \varrho \qquad \text{(by Condition (1))} \\ \text{iff} & \mathcal{B} \models \mathrm{sph}_\varrho[b_{i_1}, \ldots, b_{i_m}]. \end{array}$$

(b) Suppose that $\exists^{>k} y\ \mathrm{sph}_\tau(y)$ is a counting-sentence occuring in $\psi(\overline{x})$ with $k < T + (n{+}q) \cdot \nu_d(r)$ and a σ-type τ with radius $\leq r$ and one centre. The following equivalences hold:

$$\begin{array}{ll} & \mathcal{A} \models \exists^{>k} y\ \mathrm{sph}_\tau(y) \\ \text{iff} & |\tau(\mathcal{A})| \ \geq \ k+1 \\ \text{iff} & |\tau(\mathcal{B})| \ \geq \ k+1 \qquad (\star) \\ \text{iff} & \mathcal{B} \models \exists^{>k} y\ \mathrm{sph}_\tau(y). \end{array}$$

For Equivalence $(\star)$, assume that $|\tau(\mathcal{A})| \neq |\tau(\mathcal{B})|$. Then, by Condition (3),

$$|\tau(\mathcal{A})|, |\tau(\mathcal{B})| \ \geq \ T + (n{+}q) \cdot \nu_d(r) \ \geq \ k+1.$$

(c) Let $\exists^{\equiv k \bmod p} y\ \mathrm{sph}_\tau(y)$ be a counting-sentence occurring in $\psi(\overline{x})$ where $p \geq 2$, $k \in [0, p)$, and τ is a σ-type with radius $\leq r$ and one centre.

Since M is a multiple of p, the following equivalences hold:

$$\begin{array}{llll} & \mathcal{A} \models \exists^{\equiv k \bmod p} y \; \mathrm{sph}_\tau(y) & & \\ \text{iff} & |\tau(\mathcal{A})| \equiv k \mod p & & \\ \text{iff} & |\tau(\mathcal{B})| \equiv k \mod p & & \text{(by Condition (2))} \\ \text{iff} & \mathcal{B} \models \exists^{\equiv k \bmod p} y \; \mathrm{sph}_\tau(y). & & \end{array}$$

This completes the proof of Claim 1 and also the proof of Theorem 3.3.1. □

3.4 Model-Checking

In Section 3.2, it was shown that for each degree bound $d \geq 2$ and every relational signature σ, any formula from FO+un$\mathsf{M}[\sigma]$ can be turned effectively into a d-equivalent HNF-formula from FO+un$\mathsf{M}[\sigma]$.

As an immediate application, we obtain that Seese's fixed-parameter tractability result for model-checking of formulas from FO on structures of bounded degree [See96] can be generalised to FO+un$\mathsf{M}$. More precisely, we prove the following theorem:

Theorem 3.4.1. *There is an algorithm which, on input of*

- *a formula $\varphi(\overline{x})$ from* FO+un$\mathsf{M}$ *where $\overline{x}$ are the $n \geq 0$ free variables of φ,*
- *a finite σ-structure $\mathcal{A}$ (where σ consists of precisely the relation symbols that occur in φ), and a tuple $\overline{a} \in A^n$,*

decides whether $\mathcal{A} \models \varphi[\overline{a}]$.

This algorithm takes time in

$$(2\max\{1, T, P\})^{(||\varphi|| \cdot \nu_d(4^q))^{\mathcal{O}(||\sigma||)}} \cdot ||\mathcal{A}||$$

where $T, P, q \geq 0$ are the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$, respectively, and where $d \geq 2$ is a bound on the degree of $\mathcal{A}$.

Remark 3.4.2. Since $T, P, q, ||\sigma|| < ||\varphi||$, the algorithm of Theorem 3.4.1 takes 3-fold exponential time

$$2^{d^{2^{\mathcal{O}(||\varphi||)}}} \cdot ||\mathcal{A}||$$

in the size of φ for every σ-structure $\mathcal{A}$ with degree $d \geq 3$, and 2-fold exponential time

$$2^{2^{\mathrm{poly}(||\varphi||)}} \cdot ||\mathcal{A}||$$

in the size of φ for every σ-structure $\mathcal{A}$ with degree $d \leq 2$.

In [FG04], a different approach to such a fixed-parameter tractable model-checking algorithm for FO on structures of bounded degree is presented. This approach also uses Hanf-locality but not by constructing Hanf normal form. Note that the corresponding lower bounds, also provided in [FG04], imply that the model-checking algorithm of Theorem 3.4.1 is basically worst-case optimal (under the complexity theoretic assumption $\mathrm{FPT} \neq \mathrm{AW}[*]$).

Proof of Theorem 3.4.1. Let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)$, for a suitable $D \subseteq D_{\mathrm{all}}$, and let σ consist of precisely the relation symbols that occur in φ. Let $n := |\overline{x}|$ be the number of free variables of φ. Moreover, let $\mathcal{A}$ be a finite σ-structure and let $\overline{a} \in A^n$.

For checking whether $\mathcal{A} \models \varphi[\overline{a}]$, the algorithm proceeds as follows:

(Step 1) Compute an upper bound $d \geq 2$ on the degree of $\mathcal{A}$.

(Step 2) Employ the algorithm from Theorem 3.2.1 to transform $\varphi(\overline{x})$ into a d-equivalent HNF-formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$.

(Step 3) For each sphere-formula α that occurs in ψ, check if $\mathcal{A} \models \alpha[\overline{a}]$, and replace each occurrence of α in ψ with the Boolean constant $\mathbf{1}$ if $\mathcal{A} \models \alpha[\overline{a}]$, and with the Boolean constant $\mathbf{0}$ otherwise.

(Step 4) For each counting-sentence χ that occurs in ψ, check if $\mathcal{A} \models \chi$, and replace each occurrence of χ in ψ with the Boolean constant $\mathbf{1}$ if $\mathcal{A} \models \chi$, and with the Boolean constant $\mathbf{0}$ otherwise.

(Step 5) After having performed Steps (1) to (4), we have obtained a Boolean combination of the Boolean constants $\mathbf{0}$ and $\mathbf{1}$. Evaluate this Boolean combination and output "yes" if the result is $\mathbf{1}$, and output "no" if the result is $\mathbf{0}$.

Obviously, the algorithm's output is "yes" if, and only if, $\mathcal{A} \models \varphi[\overline{a}]$.

Time complexity. We describe the details of Steps (1) to (5) in a run time analysis of the algorithm sketched above. For the following, let $\overline{x} = (x_1, \ldots, x_n)$ and let $\overline{a} = (a_1, \ldots, a_n)$. Furthermore, let $T, P, q \geq 0$ be the threshold, the maximum period, and the quantifier rank of φ, respectively.

In the following, we abbreviate $N := ||\varphi|| \cdot \nu_d(4^q)$.

(Step 1) To compute d, compute an adjacency list representation of $\mathcal{A}$'s Gaifman-graph $\mathcal{G}_{\mathcal{A}}$: For each relation symbol R in σ and each occurrence of an

element of A in a tuple of $R^{\mathcal{A}}$, we have to add at most $\mathrm{ar}(R) \leq ||\sigma||$ edges to $\mathcal{G}_{\mathcal{A}}$. Since $\mathcal{A}$ is d-bounded, each adjacency list has $< d$ entries.

In summary, computing $\mathcal{G}_{\mathcal{A}}$ and d takes time in

$$\mathcal{O}(||\sigma||) \cdot ||\mathcal{A}|| \cdot d. \tag{1}$$

(Step 2) According to Theorem 3.2.1, the construction of the HNF-formula $\psi(\overline{x})$ takes time in

$$(2\max\{1, T, P\})^{N^{\mathcal{O}(||\sigma||)}}. \tag{2}$$

Recall that $\psi(\overline{x})$ is a Boolean combination of

(a) sphere-formulae of the shape $\mathrm{sph}_{\varrho}(\overline{x}')$, for a tuple of $m \in [1, n]$ variables belonging to the tuple $\overline{x}$ and a d-bounded σ-type ϱ with radius $\leq 4^q$ and m centres, and

(b) counting-sentences of the shape $(\mathsf{Q}{+}k)y\ \mathrm{sph}_{\tau}(y)$, with $\mathsf{Q} \in D \cup \{\exists\}$, $k \geq 0$, and a d-bounded σ-type τ with radius $\leq 4^q$ and one centre.

(Step 3) Consider a sphere-formula $\alpha(\overline{x}') \coloneqq \mathrm{sph}_{\varrho}(\overline{x}')$ with $m \in [1, n]$ free variables $\overline{x}' = (x_{i_1}, \ldots, x_{i_m})$ for suitable indices $i_1, \ldots, i_m$ from $[1, n]$, and where ϱ is a d-bounded σ-type with radius $r \leq 4^q$ and m centres.

To decide whether $\mathcal{A} \models \alpha[\overline{a}']$, for $\overline{a}' = (a_{i_1}, \ldots, a_{i_m})$, we have to check whether $\mathcal{N}_r^{\mathcal{A}}(\overline{a}') \cong \varrho$. Since $r \leq 4^q$ and $m \leq n$, this can in time

$$2^{\mathcal{O}(||\sigma||) \cdot N^2} \quad \subseteq \quad 2^{N^{\mathcal{O}(||\sigma||)}} \tag{3}$$

by using the algorithm of Lemma 2.8.6.

(Step 4) Consider a counting-sentence $\chi \coloneqq (\mathsf{Q}{+}k)y\ \mathrm{sph}_{\tau}(y)$ that occurs in ψ. In particular, τ is a d-bounded type with radius $r \leq 4^q$ and one centre.

To decide whether $\mathcal{A} \models \chi$, we first compute the number k_τ of elements $a \in A$ with $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \tau$. Afterwards, we check if $k_\tau \in (\mathsf{Q}{+}k)$. The latter can be done easily using the encoding of $(\mathsf{Q}{+}k)$.

To compute k_τ, we consider every $a \in A$, compute the sphere $\mathcal{N}_r^{\mathcal{A}}(a)$, and check whether $\mathcal{N}_r^{\mathcal{A}}(a) \cong \tau$. From Step (3) we know that for each $a \in A$ this can be done in time $2^{N^{\mathcal{O}(||\sigma||)}}$.

Since there are at most $||\psi||$ counting-sentences in ψ, the entire Step (4) takes time in

$$\begin{aligned} & (2\max\{1, T, P\})^{N^{\mathcal{O}(||\sigma||)}} \cdot 2^{N^{\mathcal{O}(||\sigma||)}} \cdot |A| \\ \subseteq \quad & (2\max\{1, T, P\})^{N^{\mathcal{O}(||\sigma||)}} \cdot |A|. \end{aligned} \tag{4}$$

(Step 5) Evaluation the resulting variable-free propositional formula takes time polynomial in the size of ψ, that is, time in

$$(2\max\{1, T, P\})^{N^{\mathcal{O}(||\sigma||)}}. \tag{5}$$

In summary, we can conclude from Estimates (1) to (5) that the total running time of the algorithm is

$$(2\max\{1, T, P\})^{N^{\mathcal{O}(||\sigma||)}} \cdot ||\mathcal{A}|| \quad = \quad (2\max\{1, T, P\})^{(||\varphi||\cdot\nu_d(4^q))^{\mathcal{O}(||\sigma||)}} \cdot ||\mathcal{A}||.$$

This completes the proof of Theorem 3.4.1. □

3.5 Conclusion

In this chapter, a generalisation of Hanf normal form to extensions of first-order logic by unary counting quantifiers was introduced. This motivated the question, which sets of unary counting quantifiers actually permit Hanf normal form. That is, for which such extensions of first-order logic by unary counting quantifiers, every formula has a d-equivalent HNF-formula for every degree bound $d \geq 0$?

As a partial answer to this question, we have shown that each logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)$, for any set $D \subseteq D_{\mathrm{all}}$, permits Hanf normal form. This extends slightly on Nurmonen's locality theorem, which only implies that $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(\{\mathsf{D}_p\})$ for single modulo-counting quantifiers permits Hanf normal form, and also lead to an alternative proof of Nurmonen's locality theorem [Nur00].

Moreover, our corresponding proof does not only show the existence of Hanf normal forms, but also how to compute them in 3-fold exponential time in the size of the input formula for degree bounds $d \geq 3$, and in 2-fold exponential time for $d = 2$. In Section 9.3, we will see that this algorithm is basically worst-case optimal for both cases.

As an application, we used our construction of Hanf normal form for a model-checking algorithm which decides whether a d-bounded interpretation $(\mathcal{A}, \overline{a})$ satisfies a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ in 3-fold (2-fold) exponential time in the size of φ, for $d \geq 3$ ($d = 2$), and in linear time in the size of $\mathcal{A}$.

In Section 7.3 and Section 8.4, we will extend the results of this chapter to further logics. In particular, in Section 7.3, we consider the extension $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ of $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ by tuple-counting quantifiers. In Section 8.4, we look beyond modulo-counting quantifiers and provide a characterisation of all sets of unary counting-quantifiers that permit Hanf normal form, answering the question stated above. More precisely, we will show that ultimately periodic logics are precisely the logics that permit Hanf normal form. Moreover, for all ultimately periodic logics, we also obtain corresponding generalisations for the algorithmic results of this chapter.

4 Gaifman Normal Form

This chapter is based on [HKS13]. It is know that the construction of an equivalent Gaifman normal form from an FO-formula involves a non-elementary blow-up, even on classes of trees of unbounded degree [DGKS07]. In contrast, for cases where only equivalence on a class of structures of degree at most d is required, this chapter presents an algorithm which computes Gaifman normal form in worst-case optimal 3-fold exponential time, for $d \geq 3$.

4.1 Introduction

In this chapter we turn our attention to Gaifman's locality theorem [Gai82] and the corresponding local normal form for first-order logic, called *Gaifman normal form*. According to [Gai82] every FO-sentence over a relational signature is equivalent to a Gaifman normal form, that is, a Boolean combination of expressions of the form

> *"there are at least k elements x of pairwise distance $> 2r$ whose r-sphere satisfies a formula $\varrho(x)$".*

However, this Gaifman normal form may be non-elementarily larger then the original formula, even when equivalence to the original formula is only required on the class of trees [DGKS07]. This non-elementary lower bound does not hold when imposing restrictions on the degree of the trees in the class.

We present an algorithm that transforms formulae from $\mathsf{FO}+\mathrm{un}\mathsf{T}$, for degree bounds $d \geq 2$, into d-equivalent formulae in Gaifman normal form from $\mathsf{FO}+\mathrm{un}\mathsf{T}$. For $d = 2$, the algorithm takes 2-fold exponential time in the size of the input formula and for $d \geq 3$, it takes 3-fold exponential time. The algorithm was published in [HKS13]. A lower bound, presented in Section 9.4, shows that it is worst-case optimal.

Our algorithm is carried out in two phases: First, the input formula is turned into a d-equivalent Hanf normal form. In a second step, all counting-sentences in this Hanf normal form are turned into equivalent sentences in Gaifman normal form.

The argument used in the second step is of independent interest: it actually shows that every formula expressing that *"there are at least k elements x that satisfy an r-local formula $\varrho(x)$"* can be transformed in 1-fold exponential time into a Gaifman normal form that is not only equivalent to it on structures of degree $\leq d$, but on all structures.

Before stating the main result of this chapter, we give a precise definition of Gaifman normal form and introduce some related notation. For this, we let σ denote a relational signature.

Definition 4.1.1. An $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$-formula $\varrho(\overline{x})$ with a non-empty set of free variables among the $n \geq 1$ variables from the tuple $\overline{x} = (x_1, \ldots, x_n)$ is said to be *r-local (around $\overline{x}$)* for an $r \in \mathbb{N}$ if

$$\mathcal{A} \models \varrho[\overline{a}] \quad \text{iff} \quad \mathcal{A}[N_r^{\mathcal{A}}(\overline{a})] \models \varrho[\overline{a}] \quad \text{for every } \sigma\text{-structure } \mathcal{A} \text{ and all } \overline{a} \in A^n.$$

Thus, r-local formulae $\varrho(\overline{x})$ only speak about the r-sphere of $\overline{x}$. A formula $\varrho(\overline{x})$ is *local* if it is r-local around $\overline{x}$, for some $r \geq 0$.

Example 4.1.2. For each $r \geq 0$, every sphere-formula $\mathrm{sph}_\tau(\overline{x})$ with a σ-type τ of radius r is r-local around $\overline{x}$. As another example, the formula $\mathrm{dist}_{\leq 2r+1}(x, y)$ from Corollary 2.8.4 is r-local around x, y.

Definition 4.1.3. A *basic local sentence* is an $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$-sentence of the shape

$$\exists x_1 \cdots \exists x_k \left(\bigwedge_{1 \leq i < j \leq k} \mathrm{dist}(x_i, x_j) > 2r \quad \wedge \quad \bigwedge_{i=1}^{k} \varrho(x_i) \right),$$

where $k, r \geq 1$ and $\varrho(x)$ is r-local around x.

Recall that a set M of elements from a σ-structure $\mathcal{A}$ is called s-scattered, for an $s \geq 0$, if all the elements in the set have pairwise distance $> s$ in the structure $\mathcal{A}$.

Thus, the basic local sentence above is satisfied by a σ-structure $\mathcal{A}$ if and only if $\mathcal{A}$ contains a $2r$-scattered set of elements which each satisfy the r-local formula ϱ. Note that, in particular, the r-neighbourhoods of these elements are disjoint and there are also no edges in the Gaifman graph $\mathcal{G}_{\mathcal{A}}$ of $\mathcal{A}$ between elements from the r-neighbourhoods of any two distinct elements of this set.

Definition 4.1.4. An $\mathsf{FO}+\mathrm{un}\mathsf{T}[\sigma]$-formula $\psi(\overline{x})$ is said to be in *Gaifman normal form* if it is a Boolean combination of local formulae and basic local sentences.

We will speak of GNF-*formulae* and GNF-*sentences* when we mean "formula in Gaifman normal form" and "sentence in Gaifman normal form", respectively.

Remark 4.1.5. Note that, while Gaifman normal form is usually defined for plain FO (cf., e.g., [EF99]), we define Gaifman normal form here for $\mathsf{FO}+\mathrm{un}\mathsf{T}$. That is, the local formulae occurring in a GNF-formula are allowed to use threshold-counting quantifiers. The motivation for this is that the construction of Hanf normal form, used as a first step in the subsequent proof, already takes as input formulae from $\mathsf{FO}+\mathrm{un}\mathsf{T}$ and produces HNF-formulae from $\mathsf{FO}+\mathrm{un}\mathsf{T}$. However, in Remark 3.1.8 we have seen that threshold-counting quantifiers can easily be expressed in FO. In fact, the overhead of such a transformation in our algorithm described below, in order to obtain GNF-formulae from FO, would be surpressed by the $\mathcal{O}$-notation.

Example 4.1.6. The following example is due to [GW04]. Let $\tau := (E, R, B)$, where E is a binary, and R, B are unary relation symbols. The $\mathsf{FO}[\tau]$-sentence

$$\varphi \;:=\; \exists x \exists y \left(\neg E(x,y) \;\wedge\; R(x) \;\wedge\; B(y)\right).$$

is equivalent to the following GNF-sentence, where the first and the third line contain basic local sentences with $k = 1$, while the second line contains a basic local sentence with $k = 2$:

$$\begin{aligned}
&\exists x\, \exists x' \exists y \Big(\mathrm{dist}(x,x') \le 2 \;\wedge\; \mathrm{dist}(x,y') \le 2 \;\wedge\; \neg E(x',y) \;\wedge\; R(x') \;\wedge\; B(y)\Big) \\
\vee\;\; &\Big(\exists x \exists y \left(\mathrm{dist}(x,y) > 2 \;\wedge\; (R(x) \vee B(x)) \;\wedge\; (R(y) \vee B(y))\right) \\
&\quad \wedge\; \exists x\, R(x) \;\wedge\; \exists x\, B(x)\Big).
\end{aligned}$$

The precise statement of this chapter's main result reads as follows:

Theorem 4.1.7. *There is an algorithm which, on input of*

- *a degree bound $d \ge 2$,*
- *a relational signature σ, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{T}[\sigma]$,*

computes a GNF-*formula $\psi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{T}[\sigma]$ that is d-equivalent to φ.*

Furthermore, if $T, q \ge 0$ are the threshold and the quantifier rank of $\varphi(\overline{x})$, the algorithm runs in time

$$2^{((T+1)\cdot||\varphi||\cdot\nu_d(4^q))^{\mathcal{O}(||\sigma||)}}.$$

Remark 4.1.8. Suppose that σ contains only the relation symbols that actually occur in $\varphi(\overline{x})$, that is, $||\sigma|| < ||\varphi||$ and recall that also $T, q < ||\varphi||$. Then, for every degree bound $d \geq 3$, the algorithm of Theorem 4.1.7 takes 3-fold exponential time

$$2^{d^{2^{\mathcal{O}(||\varphi||)}}}$$

in the size of $\varphi(\overline{x})$. And for degree bound $d = 2$, the algorithm takes 2-fold exponential time

$$2^{2^{\mathrm{poly}(||\varphi||)}}.$$

The remainder of this chapter is devoted to the proof of Theorem 4.1.7. The first step of the proof is to turn the input formula into Hanf normal form. For this, we employ the following special case of Theorem 3.2.1 for an empty set of modulo-counting quantifiers.

Corollary 4.1.9. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *a relational signature σ, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$,*

computes a HNF*-formula $\psi^H(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ that is d-equivalent to φ.*

If $T, n, q \geq 0$ are the threshold, the number of free variables, and the quantifier rank of $\varphi(\overline{x})$, then $\psi^H(\overline{x})$ has locality radius $\leq 4^q$ and threshold

$$< \ T + (n{+}q) \cdot \nu_d(4^q).$$

Furthermore, the algorithm constructs $\psi^H(\overline{x})$ in time

$$(2\max\{1, T\})^{(||\varphi||\cdot\nu_d(4^q))^{\mathcal{O}(||\sigma||)}}.$$

Recall from Definition 3.1.9 that a HNF-formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ is a Boolean combination of sphere-formulae $\mathrm{sph}_\varrho(\overline{x})$ and counting-sentences of the shape $\exists^{\geq k} y \ \mathrm{sph}_\tau(y)$ with $k \geq 1$. On input of a degree bound $d \geq 2$, a relational signature σ, and a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$, the algorithm of Theorem 4.1.7 proceeds in the following steps:

(Step 1) The algorithm of Corollary 4.1.9 transforms φ into a d-equivalent HNF-formula $\psi^H(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$.

(Step 2) Recall that a sphere-formula with locality radius $r \geq 0$ is, in particular, r-local around its free variables. Hence, to obtain an equivalent GNF-formula from $\psi^H(\overline{x})$, it suffices to transform each counting-sentence occurring in $\psi^H(\overline{x})$ into an equivalent GNF-sentence. The details of this transformation are explained in the next section.

4.2 Gaifman Normal Form for Counting-Sentences

In this section, we in fact show a more general result that

- does not restrict attention to d-equivalence, but establishes equivalence with respect to the class of *all* σ-structures, and
- does not restrict attention to counting-sentences, but considers sentences of the form $\exists^{\geq k} y\, \varrho(y)$, where $\varrho(y)$ is an *arbitrary* formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ that is r-local around y.

Consider a formula $\varrho(x)$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$. For a σ-structure $\mathcal{A}$, we consider each element a of its universe to be coloured either *red* or *blue*, depending on whether or not $\mathcal{A} \models \varrho[a]$. We let P be a unary relation symbol that is not already present in σ, and we define a (σ, P)-structure $\mathcal{C} = (\mathcal{A}, P^{\mathcal{C}})$, which extends the σ-structure $\mathcal{A}$ by a new relation $P^{\mathcal{C}}$ such that for each $a \in A$,

$$a \in P^{\mathcal{C}} \quad \text{iff} \quad \mathcal{A} \models \varrho[a].$$

Thus, we call an element a red if it belongs to $P^{\mathcal{C}}$, and blue otherwise. Note that, when evaluated in $\mathcal{A}$, the sentence $\exists^{\geq k} y\, \varrho(y)$ with $k \geq 1$ then states that $\mathcal{C}$ has at least k red elements. It is important to note that, due to $P^{\mathcal{C}}$ being a unary relation, $\mathcal{A}$ and $\mathcal{C}$ have precisely the same Gaifman graph.

The following lemma tells us about the distribution of red elements (that is, elements in $P^{\mathcal{C}}$) in (σ, P)-structures $\mathcal{C}$. This provides information that will be useful for constructing a GNF-sentence that is equivalent to $\exists^{\geq k} y\, \varrho(y)$.

Lemma 4.2.1. *Let $k, r, c \geq 1$. For every (σ, P)-structure $\mathcal{C}$, one of the following statements is true:*

(A) There is no red element in $\mathcal{C}$.

(B) $\mathcal{C}$ contains a $(c \cdot r)$-scattered set of at least k red elements.

(C) *There is a unique $\ell \in [1,k)$ such that $\mathcal{C}$ contains a $(c \cdot r)$-scattered set of ℓ red elements, but no $(c \cdot r)$-scattered set of more than ℓ red elements, and there is a non-empty set W of at most ℓ red elements such that for $s \coloneqq \ell - |W|$ and $R_s \coloneqq (c{+}1)^s \cdot c \cdot r$ the following is true:*
- *W is a $(c \cdot R_s)$-scattered set, and*
- *every red element of $\mathcal{C}$ belongs to $N^{\mathcal{C}}_{R_s}(W)$.*

Proof. It suffices to consider the case where neither Statement (A) nor Statement (B) is true. Our goal is to show that in this case Statement (C) holds.

Since neither Statement (A) nor Statement (B) is true, there is an $\ell \in [1,k)$ such that $\mathcal{C}$ contains a $(c \cdot r)$-scattered set of ℓ red elements, but no $(c \cdot r)$-scattered set of more than ℓ red elements. It remains to show that a set W of red nodes exists which satisfies Statement (C).

Towards this aim, we let $R_j \coloneqq (c{+}1)^j \cdot c \cdot r$ for all $j \in \mathbb{N}$ and proceed inductively by constructing a sequence with length $s \in [0,\ell]$ of finite sets

$$W_0 \ \supset \ W_1 \ \supset \ W_2 \ \supset \ \cdots \ \supset \ W_s$$

such that $W \coloneqq W_s$ satisfies Statement (C), and for every $j \in [0,s]$, the set W_j is of size $\ell - j$ and every red element of $\mathcal{C}$ belongs to $N^{\mathcal{C}}_{R_j}(W_j)$.

For $j = 0$, let W_0 be a $(c \cdot r)$-scattered set of ℓ red elements. By our choice of ℓ, the set $N^{\mathcal{C}}_{c \cdot r}(W_0)$ contains *all* red elements of $\mathcal{C}$ (otherwise, there would be a red node a such that $W_0 \cup \{a\}$ is a $(c \cdot r)$-scattered set of size $\ell + 1$).

In the following, consider a $j \geq 0$ and assume that the sets $W_0, \ldots, W_j$ are already constructed. Note that, if the set W_j is $(c \cdot R_j)$-scattered, we can terminate the construction by letting $s \coloneqq j$ and $W \coloneqq W_j$.

Otherwise, there are elements a and b in W_j with distance at most $c \cdot R_j$. We construct the set W_{j+1} by removing the element b from W_j, that is, we let $W_{j+1} \coloneqq W_j \setminus \{b\}$. Note that $N^{\mathcal{C}}_{R_j}(b) \subseteq N^{\mathcal{C}}_{(c+1) \cdot R_j}(a)$. As $R_{j+1} = (c{+}1) \cdot R_j$, we thus know that every red node of $\mathcal{C}$ belongs to $N^{\mathcal{C}}_{R_{j+1}}(W_{j+1})$.

Since $|W_j| = \ell - j$, the construction ends after at most $\ell - 1$ steps, resulting in a set W with the desired properties. $\square$

Note that similar results to Lemma 4.2.1 have been used before, cf. e.g. Claim 4.4 in [ADG08] and Lemma 8 in [DGKS06].

We can use Lemma 4.2.1 to show the following technical result, which is the key lemma that enables us to find an appropriate GNF-sentence that is equivalent to the sentence $\exists^{\geq k} y\, \varrho(y)$, provided that ϱ is local around x for some $r \geq 0$.

Lemma 4.2.2. *Let $\mathcal{C}$ be a (σ, P)-structure, let $r \geq 1$, and let $R_s \coloneqq 9^s \cdot 8r$ for all $s \in \mathbb{N}$.*

For each $k \geq 1$, $\mathcal{C}$ contains at least k red elements if and only if one of the following statements is true:

(1) $\mathcal{C}$ contains an $8r$-scattered set of at least k red elements.

(2) There is a red element in $\mathcal{C}$ whose R_k-neighbourhood contains at least k red elements.

(3) Each of the following statements is true:

(i) There is a unique $\ell \in [1, k)$ such that $\mathcal{C}$ contains an $8r$-scattered set of ℓ red elements, but no $8r$-scattered set of more than ℓ red elements.

(ii) There is an $s \in [0, \ell)$ such that $\mathcal{C}$ contains an $8R_s$-scattered set of $\ell - s$ red elements and if $s \geq 1$, then $\mathcal{C}$ does not contain an $8R_{s-1}$-scattered set of $\ell - (s-1)$ red elements.

(iii) There is a number $t \in [1, \ell - s]$ and numbers

$$1 \leq n_1 < \cdots < n_t < k \quad \text{and} \quad m_1, \ldots, m_t \in [1, k]$$

with

$$m_1 + \cdots + m_t \;=\; \ell - s \quad \text{and} \quad m_1 \cdot n_1 + \cdots + m_t \cdot n_t \;\geq\; k$$

such that for each $j \in [1, t]$ there is a $6R_s$-scattered set of m_j red elements whose $2R_s$-neighbourhoods each contain exactly n_j red elements.

Proof. We prove the two directions of Lemma 4.2.2.

For the "only if" direction, suppose that $\mathcal{C}$ contains at least k red nodes. It suffices to consider the case where neither Statement (1) nor Statement (2) is true. Our goal is to show that in this case Statement (3), that is, each of the Statements (3.i) to (3.iii), is satisfied.

We use Lemma 4.2.1 for the numbers k and r, and we let $c \coloneqq 8$. Note that by assumption, $\mathcal{C}$ does not satisfy Statement (A) of Lemma 4.2.1. Moreover, by choice of the number $c = 8$, $\mathcal{C}$ also does not satisfy Statement (B) of Lemma 4.2.1. Thus, Statement (C) of Lemma 4.2.1 must be true:

- There is an $\ell \in [1, k)$ such that $\mathcal{C}$ contains an $8r$-scattered set of ℓ red elements, but no $8r$-scattered set of more than ℓ red elements, and hence, *Statement (3.i) is satisfied.*

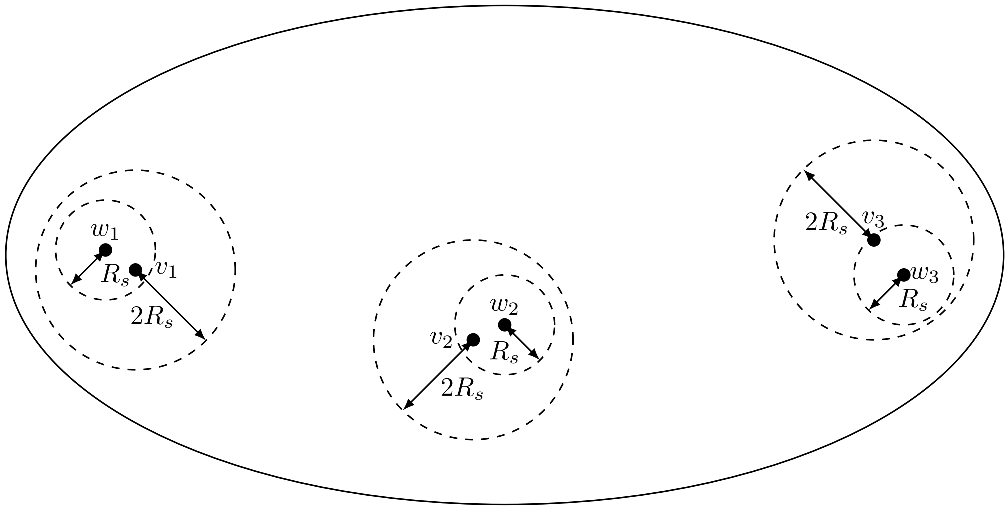

Figure 4.1 Illustration for Lemma 4.2.2 with $\ell - s = 3$. All red nodes of $\mathcal{C}$ belong to the R_s-neighbourhood of the elements w_i, and thus to the $2R_s$-neighbourhood of the elements v_i, for $i \in \{1, 2, 3\}$. The elements w_i have pairwise distance $> 8R_s$.

- There is a number $s \in [0, \ell)$ and an $8R_s$-scattered set W of $\ell - s$ red elements $w_1, \ldots, w_{\ell-s}$ such that $N^{\mathcal{C}}_{R_s}(W)$ contains all red elements of $\mathcal{C}$. For the following, we choose the number $s \in [0, \ell)$ minimal such that the above holds. In particular, *Statement (3.ii) is satisfied.*

It remains to show that Statement (3.iii) also holds. For every $i \in [1, \ell{-}s]$ let $n_i \in \mathbb{N}_{\geq 1}$ be the number of red elements in $N^{\mathcal{C}}_{R_s}(w_i)$. Since $N^{\mathcal{C}}_{R_s}(w_i) \subseteq N^{\mathcal{C}}_{R_k}(w_i)$ and, by assumption, Statement (2) does not hold, we know that also $n_i \in [1, k)$.

Let us summarise the information we have collected until now (see Figure 4.1 for an illustration):

- The set W is $8R_s$-scattered. That is, for all distinct $i, j \in [1, \ell{-}s]$, the elements w_i and w_j have $\mathrm{dist}^{\mathcal{C}}(w_i, w_j) > 8R_s$.
- Every red element of $\mathcal{C}$ belongs to $N^{\mathcal{C}}_{R_s}(\{w_1, \ldots, w_{\ell-s}\})$. Recall that, by assumption, $\mathcal{C}$ contains at least k red elements. Thus, it follows that

$$n_1 + \cdots + n_{\ell-s} \;\geq\; k.$$

- For all distinct $i, j \in [1, \ell{-}s]$ and for all $v_i \in N^{\mathcal{C}}_{R_s}(w_i)$ and $v_j \in N^{\mathcal{C}}_{R_s}(w_j)$ we have $\mathrm{dist}^{\mathcal{C}}(v_i, v_j) > 6R_s$.

- For each $i \in [1, \ell{-}s]$ and every $v_i \in N^{\mathcal{C}}_{R_s}(w_i)$, the set $N^{\mathcal{C}}_{2R_s}(v_i)$ contains exactly the same red elements as $N^{\mathcal{C}}_{R_s}(w_i)$.

Let us now group the numbers $n_1, \ldots, n_{\ell-s}$ according to their value. To this end, let $T := \{n_1, \ldots, n_{\ell-s}\}$ be the set of distinct values among the numbers $n_1, \ldots, n_{\ell-s}$ and let $t := |T|$ be the number of distinct values. For each value in T, we choose a representative among the numbers $n_1, \ldots, n_{\ell-s}$ with this value. That is, we choose indices $i_1, \ldots, i_t \in [1, \ell{-}s]$ such that $T = \{n_{i_1}, \ldots, n_{i_t}\}$. For each $j \in [1, t]$, we let

$$m_{i_j} \quad := \quad |\{i \in [1, \ell{-}s] \,:\, n_i = n_{i_j}\}|$$

be the number of occurrences of the value n_{i_j} among the numbers $n_1, \ldots, n_{\ell-s}$. Then *Statement (3.iii) is satisfied*, since

$$m_{i_1} + \cdots + m_{i_t} \;=\; \ell{-}s$$

and

$$m_{i_1} \cdot n_{i_1} + \cdots + m_{i_t} \cdot n_{i_t} \;=\; n_1 + \cdots + n_{\ell-s} \;\geq\; k,$$

and furthermore, for every $j \in [1, t]$, there are is a $6R_s$-scattered set of at least m_{i_j} red elements whose $2R_s$-neighbourhoods each contain exactly n_{i_j} red elements. This completes the proof of the "only if" direction of Lemma 4.2.2.

For the "if" direction, observe that if Statement (1) or Statement (2) is true, then $\mathcal{C}$ obviously contains at least k red elements. Hence, in the following we suppose that Statement (3) is satisfied. In this case it follows from Statement (3.i) that there is an $8r$-scattered set of red elements, but no $8r$-scattered set of more than ℓ red elements.

Moreover, according to Statement (3.ii), there is a number $s \in [0, \ell)$ and an $8R_s$-scattered set of red elements $w_1, \ldots, w_{\ell-s}$, for which the following claims are true:

Claim 1. *All red elements of $\mathcal{C}$ belong to $N^{\mathcal{C}}_{R_s}(\{w_1, \ldots, w_{\ell-s}\})$.*

For a *proof of Claim 1*, assume towards a contradiction that there is a red element $v \notin N_{R_s}(\{w_1, \ldots, w_{\ell-s}\})$. If $s = 0$, then $\{w_1, \ldots, w_\ell, v\}$ is a $8r$-scattered set of $\ell + 1$ red nodes, contradicting Statement (3.i). In case that $s > 0$ we know that $\mathrm{dist}^{\mathcal{C}}(v, w_i) > R_s = 9R_{s-1} > 8R_{s-1}$, for all $i \in [1, \ell{-}s]$. Thus, there is an $8R_{s-1}$-scattered set of $(\ell{-}s) + 1 = \ell - (s{-}1)$ red elements. This contradicts the choice of s according to Statement (3.ii).

The following claim holds, since for all distinct $i, j \in [1, \ell{-}s]$, we have $\mathrm{dist}^{\mathcal{C}}(w_i, w_j) > 8R_s$.

Claim 2. *For all distinct $i, j \in [1, \ell{-}s]$ and for all nodes $v_i \in N^{\mathcal{C}}_{R_s}(w_i)$ and $v_j \in N^{\mathcal{C}}_{R_s}(w_j)$, we have $\mathrm{dist}^{\mathcal{C}}(v_i, v_j) > 6R_s$.*

As an immediate consequence of Claim 1 and Claim 2 we obtain

Claim 3. *For each $i \in [1, \ell{-}s]$ and every $v_i \in N^{\mathcal{C}}_{R_s}(w_i)$, the $2R_s$-neighbourhood of v_i contains exactly the same red elements as the R_s-neighbourhood of w_i.*

From Statement (3.iii) we know that there is a number $t \in [1, \ell{-}s]$ and numbers

$$1 \leq n_1 < \cdots < n_t < k \qquad \text{and} \qquad m_1, \ldots, m_t \in [1, k]$$

with

$$m_1 + \cdots + m_t \;=\; \ell{-}s \qquad \text{and} \qquad m_1 \cdot n_1 + \cdots + m_t \cdot n_t \;\geq\; k \tag{1}$$

such that for each $j \in [1, t]$ there is a $6R_s$-scattered set of m_j red elements $u_{j,1}, \ldots, u_{j,m_j}$ whose $2R_s$-neighbourhoods each contain exactly n_j red elements.

Due to Claim 1, for each of the red elements $u_{j,i}$ there exists a number $k_{j,i} \in [1, \ell{-}s]$ such that $u_{j,i} \in N^{\mathcal{C}}_{R_s}(w_{k_{j,i}})$. The following claim implies that each of the nodes $u_{j,i}$ belongs to the R_s-neighbourhood of a different element from $w_1, \ldots, w_{\ell-s}$.

Claim 4. *For all $j, j' \in [1, t]$ and $i \in [1, m_j]$, $i' \in [1, m_{j'}]$, it holds that*

$$\textit{if} \quad k_{j,i} = k_{j',i'} \quad \textit{then} \quad j = j' \quad \textit{and} \quad i = i'.$$

We will prove Claim 4 below. Since $w_1, \ldots, w_{\ell-s}$ form an $8R_s$-scattered set, Claim 4 in particular implies that the $2R_s$-neighbourhoods for each of the nodes $u_{j,i}$ do not intersect. By Property (1), that is, Statement (3.iii), we thus obtain that there are indeed $m_1 \cdot n_1 + \cdots + m_t \cdot n_t \geq k$ distinct red elements in $\mathcal{C}$.

Thus we have shown that $\mathcal{C}$ has at least k red elements. With the proof of Claim 4 below, the proof of the "if" direction and also the whole proof of Lemma 4.2.2 are complete.

Proof of Claim 4. Let $\kappa := k_{j,i} = k_{j',i'}$ and observe that the nodes $u_{j,i}$ and $u_{j',i'}$ both belong to the R_s-neighbourhood of w_κ. Thus, their distance is at most $2R_s$. From Claim 3 we know that the $2R_s$-neighbourhood of $u_{j,i}$ contains exactly the same red elements as the $2R_s$-neighbourhood of $u_{j',i'}$. Thus $n_j = n_{j'}$, and hence $j = j'$. Consequently $i = i'$, for otherwise the distance of $u_{j,i}$ and $u_{j,i'}$ would be larger than $6R_s$. $\square$

We are now ready to prove this section's main result.

Theorem 4.2.3. *There is an algorithm which, on input of*

- *a relational signature* σ,
- *numbers* $k, r \geq 1$, *and*
- *a formula* $\varrho(y)$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ *that is* r*-local around* y,

computes a GNF*-sentence* ψ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ *that is equivalent to the formula* $\exists^{\geq k} y\, \varrho(y)$ *on the class of all* σ*-structures.*

Furthermore, the algorithm constructs ψ *in time*

$$2^{\mathcal{O}(k \cdot \log k)} \cdot (||\sigma|| \cdot \log r + ||\varrho||).$$

Proof. Let σ be a relational signature, let $k, r \geq 1$, and let $\varrho(y)$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ that is r-local around y. The GNF-sentence ψ is obtained by a direct translation of the Statements (1) to (3) of Lemma 4.2.2 into a Boolean combination of basic local sentences. To estimate the time needed for performing this construction, we explicitly spell out the translation and provide upper bounds on the size of the formulae involved (for all of these formulae, it is easy to see that the time required for their construction is bounded by their size, up to a constant factor). The following notation will be useful:

- For all $K \geq 1$, $R > r$, and every formula $\gamma(y)$ that is r-local around y,

  $$\chi_R^K(\gamma) \quad \coloneqq \quad \exists x_1 \cdots \exists x_K \left(\bigwedge_{1 \leq i < j \leq K} \mathrm{dist}(x_i, x_j) > 2R \quad \wedge \quad \bigwedge_{i=1}^{K} \gamma(x_i) \right)$$

  is a basic local sentence. By Corollary 2.8.4, there is a number $c_1 \in \mathbb{N}_{\geq 1}$ such that

  $$||\chi_R^K(\gamma)|| \quad \leq \quad c_1 \cdot (K^2 \cdot ||\sigma|| \cdot \log R + K \cdot ||\gamma||). \tag{1}$$

- Furthermore, for every $n \geq 1$,

  $$\begin{aligned} \lambda_R^n(x) \ &\coloneqq \ \varrho(x) \ \wedge \ \exists^{\geq n} y \left(\mathrm{dist}(x, y) \leq R \ \wedge \ \varrho(y)\right) \qquad \text{and} \\ \lambda_R^{=n}(x) \ &\coloneqq \ \lambda_R^n(x) \ \wedge \ \neg \lambda_R^{n+1}(x) \end{aligned}$$

  are $(R{+}r)$-local around x, and there is a number $c_2 \in \mathbb{N}_{\geq 1}$, such that

  $$||\lambda_R^n||, ||\lambda_R^{=n}|| \quad \leq \quad c_2 \cdot (n + ||\sigma|| \cdot \log R + ||\varrho||). \tag{2}$$

We now let

$$\psi \ := \ \psi_1 \ \vee \ \psi_2 \ \vee \ \psi_3$$

where, for each $j \in \{1,2,3\}$, ψ_j is a formalisation of Statement (j) of Lemma 4.2.2. More precisely, we let $R_s := 9^s \cdot 8r$ for $s \in \mathbb{N}$, and we let

$$\psi_1 \ := \ \chi^k_{4r}(\varrho) \quad \text{and} \quad \psi_2 \ := \ \exists x\, \lambda^k_{R_k}(x).$$

By Estimate (1) and since $4r < R_k$, there is a number $c_3 > c_1$, such that

$$||\psi_1||, ||\psi_2|| \quad \leq \quad c_3 \cdot (k^2 \cdot ||\sigma|| \cdot \log R_k + k \cdot ||\varrho||).$$

The formula ψ_3 is chosen as follows:

$$\psi_3 \ := \ \bigvee_{\ell=1}^{k-1} \bigvee_{s=0}^{\ell-1} \big(\chi^\ell_{4r}(\varrho) \ \wedge \ \neg\chi^{\ell+1}_{4r}(\varrho) \ \wedge \ \vartheta_{\ell,s} \ \wedge \ \xi_{\ell,s}\big),$$

where for each $\ell \in [1,k)$,

$$\begin{aligned} \vartheta_{\ell,0} \ &:= \ \chi^\ell_{4R_0}(\varrho) && \text{and} \\ \vartheta_{\ell,s} \ &:= \ \chi^{\ell-s}_{4R_s}(\varrho) \ \wedge \ \neg\chi^{\ell-(s-1)}_{4R_{s-1}}(\varrho), && \text{for } s \in [1,\ell), \text{ and} \\ \xi_{\ell,s} \ &:= \ \bigvee_{t=1}^{\ell-s} \bigvee_{D_{\ell,s,t}} \bigwedge_{j=1}^{t} \chi^{m_j}_{3R_s}\big(\lambda^{=n_j}_{2R_s}(x)\big), && \text{for } s \in [0,\ell). \end{aligned}$$

In the latter formula, the expression "$\bigvee_{D_{\ell,s,t}}$" denotes the disjunction over all possible choices of numbers $1 \leq n_1 < \cdots < n_t < k$ and $m_1, \ldots, m_t \in [1,k]$ such that

$$m_1 + \cdots + m_t \ = \ \ell{-}s \quad \text{and} \quad m_1 \cdot n_1 + \cdots + m_t \cdot n_t \ \geq \ k.$$

Note that the formula $\lambda^{=n_j}_{2R_s}(x)$ is $(2R_s{+}r)$-local and thus $3R_s$-local around x. Hence, the formula $\chi^{m_j}_{3R_s}(\lambda^{=n_j}_{2R_s}(x))$ is a basic local sentence. Furthermore, also the formulae $\chi^K_R(\varrho)$ with $K \in \{\ell, \ell{+}1, \ell{-}s, \ell{-}(s{-}1)\}$ and $R \in \{4r, 4R_s, 4R_{s-1}\}$ that ψ_3 is built of, are basic local sentences. Thus, ψ is a GNF-sentence which, due to Lemma 4.2.2, is equivalent to φ on all σ-structures.

Time complexity. For an estimate on the size of ψ and on the time required for its construction it remains to estimate the size of the subformula ψ_3: For the sentences $\chi^\ell_{4r}(\varrho)$ and $\chi^{\ell+1}_{4r}(\varrho)$, observe that $\ell < k$ and $4r < R_k$. Thus,

$$||\chi^\ell_{4r}(\varrho)||, ||\chi^{\ell+1}_{4r}(\varrho)|| \quad \leq \quad c_1 \cdot (k^2 \cdot ||\sigma|| \cdot \log R_k + k \cdot ||\varrho||). \tag{3}$$

For each $s \in \mathbb{N}$ with $s < \ell < k$ we have $4R_s < R_k$. Hence, there is a number $c_4 > c_1$, such that

$$||\vartheta_{\ell,s}|| \quad \leq \quad c_4 \cdot (k^2 \cdot ||\sigma|| \cdot \log R_k + k \cdot ||\varrho||). \tag{4}$$

As $n_j < k$, the formula $\lambda_{2R_s}^{=n_j}(x)$ has size

$$||\lambda_{2R_s}^{=n_j}(x)|| \quad \leq \quad c_2 \cdot (k + ||\sigma|| \cdot \log R_k + ||\varrho||).$$

Since also $m_j \leq k$, there is a number $c_5 \geq c_1 \cdot c_2$, such that

$$||\chi_{3R_s}^{m_j}(\lambda_{2R_s}^{=n_j}(x))|| \quad \leq \quad c_5 \cdot (k^2 \cdot ||\sigma|| \cdot \log R_k + k \cdot ||\varrho||). \tag{5}$$

As $\ell - s < k$, the disjunction "$\bigvee_{D_{\ell,s,t}}$" has at most k^{2k} clauses. Hence, there is a number $c_6 \in \mathbb{N}_{\geq 1}$ such that

$$\begin{aligned} ||\xi_{\ell,s}|| \quad &\leq \quad c_6 \cdot (k \cdot k^{2k} \cdot k \cdot ||\chi_{3R_{k-2}}^{k}(\lambda_{2R_{k-2}}^{=k}(x))||) \\ &\leq \quad c_7 \cdot (k^{2k+4} \cdot ||\sigma|| \cdot \log R_k + k^{2k+3} \cdot ||\varrho||), \end{aligned} \tag{6}$$

where $c_7 \geq c_5 \cdot c_6$.

Thus, by Estimate (3), (4) and (6), there is a number $c_8 > \max\{c_4, c_7\}$ such that

$$\begin{aligned} ||\psi_3|| \quad &\leq \quad c_8 \cdot (k^2 \cdot (k^{2k+4} \cdot ||\sigma|| \cdot \log R_k + k^{2k+3} \cdot ||\varrho||)) \\ &\leq \quad c_8 \cdot (k^{2k+6} \cdot ||\sigma|| \cdot \log R_k + k^{2k+5} \cdot ||\varrho||). \end{aligned}$$

By using the estimates on the size of ψ_1, ψ_2, and ψ_3, we obtain that there are numbers $c_{10} > c_9 > \max\{c_3, c_8\}$ such that

$$\begin{aligned} ||\psi|| \quad &\leq \quad c_9 \cdot (k^{2k+6} \cdot ||\sigma|| \cdot \log R_k + k^{2k+5} \cdot ||\varrho||) \\ &\leq \quad c_{10} \cdot (k^{2k+7} \cdot ||\sigma|| \cdot \log r + k^{2k+5} \cdot ||\varrho||). \end{aligned}$$

Here, the latter inequality holds since $R_k = 9^k 8r$.

We obtain that ψ has size in

$$2^{\mathcal{O}(k \cdot \log k)} \cdot (||\sigma|| \cdot \log r + ||\varrho||).$$

Furthermore, there obviously is an algorithm which, on input of k, r, and ϱ, constructs ψ in time $2^{\mathcal{O}(k \cdot \log k)} \cdot (||\sigma|| \cdot \log r + ||\varrho||)$. This completes the proof of Theorem 4.2.3. $\square$

Recall that, by Lemma 2.8.8, for all $d \geq 2$, each $r \geq 1$, and every d-bounded σ-type of radius $\leq r$ and with a single centre, the corresponding sphere-formula $\mathrm{sph}_\tau(y)$ has size in $\nu_d(r)^{\mathcal{O}(||\sigma||)}$.

Hence, in the particular case of a sentence $\exists^{\geq k} y\, \varrho(y)$ where $\varrho(y)$ is of the form $\mathrm{sph}_\tau(y)$, for a d-bounded type of radius $\leq r$ and with a single centre, we obtain from Theorem 4.2.3 an algorithm which, on input of a counting-sentence, constructs an equivalent GNF-sentence:

Corollary 4.2.4. *There is an algorithm which, on input of a counting-sentence*

$$\varphi \;:=\; \exists^{\geq k} y\ \mathrm{sph}_\tau(y)$$

with $k \geq 1$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$, where σ consists of precisely the relation symbols that occur in φ, computes a GNF-sentence ψ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ that is equivalent to φ on all σ-structures.

The algorithm computes ψ in time

$$2^{\mathcal{O}(k \cdot \log k)} \cdot \nu_d(r)^{\mathcal{O}(||\sigma||)},$$

where $d \geq 2$ and $r \geq 1$ are upper bounds on the degree bound and the radius of the one-centred σ-type τ, respectively.

4.3 The Gaifman Normal Form Algorithm

By using Corollary 4.1.9 for the construction of HNF-formulae and Corollary 4.2.4 to transform threshold-counting sentences into GNF-sentences, we can now prove Theorem 4.1.7.

Proof of Theorem 4.1.7. We describe the algorithm on input of a degree bound $d \geq 2$, a relational signature σ, and a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ with quantifier rank $q \geq 0$, threshold $T \geq 0$, and $n \geq 0$ free variables. For this, we abbreviate $N := ||\varphi|| \cdot \nu_d(4^q)$.

The algorithm proceeds as follows:

(Step 1) Use Corollary 4.1.9 to transform $\varphi(\overline{x})$ into a d-equivalent HNF-formula $\psi^H(\overline{x})$. This takes time in

$$(2\max\{1,T\})^{N^{\mathcal{O}(||\sigma||)}},$$

and $\psi^H(\overline{x})$ has locality radius $\leq 4^q$ and threshold

$$<\; T + (n{+}q) \cdot \nu_d(4^q) \;<\; T + N.$$

(Step 2) Use Corollary 4.2.4 to transform each counting-sentence in $\psi^H(\overline{x})$ into an equivalent GNF-sentence.

Consider a counting-sentence $\exists^{\geq k} y \ \mathrm{sph}_\tau(y)$. For $k = 1$, the counting-sentence is also a basic local sentence. Thus, we only have to consider the case of $k \geq 2$. Recall that τ has locality radius $\leq 4^q$ and that $k < T + N$. From Corollary 4.2.4 we know that the construction of an equivalent GNF-sentence takes time in

$$\begin{aligned} 2^{\mathcal{O}((T+N)\cdot\log(T+N))} \cdot \nu_d(4^q)^{\mathcal{O}(||\sigma||)} \quad &\subseteq \quad 2^{\mathcal{O}((T+N)^2)} \cdot N^{\mathcal{O}(||\sigma||)} \\ &\subseteq \quad 2^{(T+N)^{\mathcal{O}(||\sigma||)}}. \end{aligned}$$

Since every sphere-formula occurring in $\psi^H(\overline{x})$ is already a local formula, this completes the construction of the GNF-formula $\psi(\overline{x})$. As also the size of $\psi^H(\overline{x})$ is bounded by $(2\max\{1,T\})^{N^{\mathcal{O}(||\sigma||)}}$, the algorithm takes altogether time in

$$(2\max\{1,T\})^{N^{\mathcal{O}(||\sigma||)}} \cdot 2^{(T+N)^{\mathcal{O}(||\sigma||)}} \quad \subseteq \quad 2^{((T+1)\cdot N)^{\mathcal{O}(||\sigma||)}}.$$

By replacing N with $||\varphi|| \cdot \nu_d(4^q)$ again, we obtain a running time in

$$2^{((T+1)\cdot||\varphi||\cdot\nu_d(4^q))^{\mathcal{O}(||\sigma||)}}$$

This completes the proof of Theorem 4.1.7. □

4.4 Conclusion

In this chapter, we have presented an algorithm that turns a formula from FO+unT into a d-equivalent Gaifman normal form. For $d \geq 3$, the algorithm has 3-fold exponential time complexity with respect to the size of the input formula, and for $d = 2$, its time complexity is 2-fold exponential. For both cases, a matching lower bound in Section 9.4 will show that the algorithm is basically worst-case optimal.

The algorithm relies on the construction of Hanf normal form, presented in Chapter 3. The crucial step of the algorithm is the construction of Gaifman normal form for counting-sentences. Towards this aim, we have shown that, more generally, for each FO+unT-formula φ of the shape $\exists^{\geq k} y \ \varrho(y)$ where ϱ is local around y, a sentence in Gaifman normal form, which is equivalent to φ on *all* structures of the respective signature, can be computed in 1-fold exponential time.

5 Feferman-Vaught Decompositions

It is known that that the construction of Feferman-Vaught decompositions for first-order formulae involves a non-elementary blow-up, even on classes of trees of unbounded degree [DGKS07]. In contrast, in this chapter, we present an algorithm that computes such decompositions with respect to disjoint sums of d-bounded structures in worst-case optimal 3-fold exponential time, for degree bounds $d \geq 3$. The algorithm also allows input formulae with modulo-counting quantifiers. For FO-formulae, we furthermore generalise the algorithm to decompositions with respect to transductions and, in particular, direct products. This chapter is based on [HHS14, HHS15].

5.1 Introduction

Algorithmic versions of decompositions à la Feferman-Vaught are typically of the following form (cf., [Mak04, GJL12]): A given sentence φ that shall be evaluated in the composition $\mathcal{A}$ of s structures $\mathcal{A}_1, \ldots, \mathcal{A}_s$, can be transformed into a sequence $\Delta_1, \ldots, \Delta_s$ of finite sets of formulae and a propositional formula β whose propositions are tests of the form

> *"the i-th structure $\mathcal{A}_i$ satisfies the j-th formula in Δ_i"*,

such that $\mathcal{A}$ is a model of φ if and only if β is true. Further down below, we will give a formal description of such decompositions in terms of so-called *reduction sequences* (cf.,e.g., [Mak04]).

In this chapter, we first focus on compositions given by disjoint sums[1] (cf., e.g., [Hod93, KM14]) of structures. Informally, a disjoint sum is a disjoint union of structures extended by additional unary relation symbols that represent the universes of the disjoint component structures, and a $\oplus$-decomposition is a decomposition with respect to such disjoint sums.

The main result of this chapter is an algorithm which computes $\oplus$-decompositions for formulae from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ on classes of structures of bounded degree.

[1] also called "rich disjoint sums" (cf., e.g., [KM14])

The algorithm takes 3-fold exponential time in the size of the input formula for degree bounds $d \geq 3$, and 2-fold exponential time for degree bound $d = 2$. For both cases, a matching lower bound (see Section 9.5) shows that the algorithm is worst-case optimal. The lower bounds for $d = 2$ and $d = 3$, as well as the algorithm for the special case of input formulae from FO, were published in [HHS14, HHS15].

In the remainder of the chapter, we consider other forms of compositions of structures apart from disjoint sums. Section 5.3 defines compositions that are obtained by applying transductions to disjoint sums, and shows how to compute corresponding decompositions in elementary time on classes of structures of bounded degree. As an example, we use this result in Section 5.4 to compute $\otimes$-decompositions, that is, decompositions with respect to direct products of structures. Note that in Section 5.3 and Section 5.4, we have to restrict ourselfs to input formulae from FO. For this case, both algorithms were already published in [HHS14, HHS15]. We will get rid of the restriction to FO later in Section 7.4.

Before turning to the proof of Theorem 5.2.1, we give formal definitions of disjoint sums of structures, reduction sequences, and $\oplus$-decompositions.

5.1.1 Disjoint Sums

Throughout the remainder of this chapter, we let σ denote a relational signature and we let $P_1, P_2, \dots$ be a sequence of unary relation symbols that are not already present in σ. For every $s \geq 1$, we let $\sigma_s := (\sigma, P_1, \dots, P_s)$ denote the extension of σ by the relation symbols $P_1, \dots, P_s$.

Disjoint sums extend disjoint unions of structures by labelling the elements of the universe according to the component structure they originate from.

Definition 5.1.1. Let $s \geq 1$, and let $\mathcal{A}_1, \dots, \mathcal{A}_s$ be σ-structures. A *disjoint sum of* $\mathcal{A}_1, \dots, \mathcal{A}_s$ is a σ_s-structure $\mathcal{S}$ with the following properties:

- The σ-reduct of $\mathcal{S}$ is a disjoint union of $\mathcal{A}_1, \dots, \mathcal{A}_s$ and thus, in particular, a union of structures $\mathcal{A}'_1, \dots, \mathcal{A}'_s$ with pairwise disjoint universes and such that there is an isomorphism $\pi_i \colon A'_i \to \mathcal{A}_i$ from $\mathcal{A}'_i$ to $\mathcal{A}_i$ for each $i \in [1, s]$.
- For each $i \in [1, s]$, the unary relation $P_i^{\mathcal{S}}$ contains precisely the elements of the universe A'_i of $\mathcal{A}'_i$.

We call $\pi_1^{-1}, \dots, \pi_s^{-1}$ *references of* $\mathcal{A}_1, \dots, \mathcal{A}_s$ *in* $\mathcal{S}$. On the other hand, the union $\pi \colon S \to A_1 \cup \dots \cup A_s$ of the functions $\pi_1, \dots, \pi_s$ (that is, the function π where $\pi(a) := \pi_i(a)$ for all $i \in [1, s]$ and $a \in A'_i$) is a *back reference of* $\mathcal{S}$ *in* $\mathcal{A}_1, \dots, \mathcal{A}_s$.

Note that, e.g., a disjoint sum of a structure with itself shows that (back) references are not uniquely determined.

Observe that the sets $P_1^{\mathcal{S}}, \ldots, P_s^{\mathcal{S}}$ in $\mathcal{S}$ form a partition of the universe S, and for all distinct $i, j \in [1, s]$ there is no edge in the Gaifman graph of $\mathcal{S}$ between any $a \in P_i^{\mathcal{S}}$ and $b \in P_j^{\mathcal{S}}$.

5.1.2 Reduction Sequences

For the following definitions, let L denote a logic as defined in Section 2.4.2..

Definition 5.1.2. For each $i \in [1, s]$, let Δ_i be a finite set of formulae δ from $\mathsf{L}[\sigma]$ and let β be a propositional formula that only uses the propositional symbols $X_{i,\delta}$ for all $i \in [1, s]$ and $\delta \in \Delta_i$. The tuple

$$\Delta \ = \ (\beta, \Delta_1, \ldots, \Delta_s)$$

is called an *s-ary reduction sequence over* $\mathsf{L}[\sigma]$ (for short: *reduction sequence*).

If the size of the formulae in the sets $\Delta_1, \ldots, \Delta_s$ is defined (e. g., if the logic L is ultimately periodic), then the size $||\Delta||$ of Δ can be defined as

$$||\beta|| \ + \ \sum_{i=1}^{s} \sum_{\delta \in \Delta_i} ||\delta||.$$

The reduction sequence Δ represents a Boolean combination of statements, expressed by formulae from the sets $\Delta_1, \ldots, \Delta_s$, about the individual structures of sequences $\mathcal{A}_1, \ldots, \mathcal{A}_s$ of σ-structures.

In the following, we define models of such reduction sequences.

Definition 5.1.3. Let $s \geq 1$ and let $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ be an s-ary reduction sequence over $\mathsf{L}[\sigma]$, where the free variables of each formula in the sets $\Delta_1, \ldots, \Delta_s$ belong to a tuple $(x_1, \ldots, x_n)$ of length $n \geq 0$.

If $\mathcal{A}_1, \ldots, \mathcal{A}_s$ are σ-structures and $a_1, \ldots, a_n$ are elements from $A_1 \cup \cdots \cup A_s$, then the tuple $(\mathcal{A}_1, \ldots, \mathcal{A}_s, (a_1, \ldots, a_n))$ is a *model of* Δ, for short

$$\mathcal{A}_1, \ldots, \mathcal{A}_s \ \models \ \Delta[a_1, \ldots, a_n],$$

if, and only if, $\mu \models \beta$, where $\mu \colon \mathsf{PS} \to \{0, 1\}$ is a propositional interpretation such that for each $i \in [1, s]$ and every formula $\delta(x_1, \ldots, x_n) \in \Delta_i$, it holds that

$$\begin{aligned} \mu(X_{i,\delta}) = 1 \quad \text{iff} \quad & a_j \in A_i \text{ for every } x_j \in \text{free}(\delta), \quad \text{and} \\ & \mathcal{A}_i \ \models \ \delta[a_1, \ldots, a_n]. \end{aligned}$$

Note that not all of the variables $x_1, \ldots, x_n$ have to be free in each formula δ.

5.1.3 Decompositions with respect to Disjoint Sums

We are now ready to define $\oplus$-decompositions as a special case of reduction sequences. For this, let L' denote a logic. Typically, in this chapter, L' and L will be the same logic FO+unM or FO, respectively. In later chapters, we will consider cases where $\mathsf{L} = \mathsf{L}'_{\mathrm{tpl}}$.

Definition 5.1.4. Let $\mathfrak{C}$ be a class of σ-structures and let $\varphi(\overline{x})$ be a formula from $\mathsf{L}'[\sigma_s]$, whose $n \geq 0$ free variables are given by the tuple $\overline{x}$.

An *s-ary $\oplus$-decomposition for $\varphi(\overline{x})$ (on $\mathfrak{C}$) over* $\mathsf{L}[\sigma]$ is an s-ary reduction sequence $\Delta = (\beta, \Delta_1, \dots, \Delta_s)$ over $\mathsf{L}[\sigma]$, where the free variables of the formulae in the sets $\Delta_1, \dots, \Delta_s$ belong to the tuple $\overline{x}$, and for which the following holds:

If $\mathcal{S}$ is a disjoint sum of σ-structures $\mathcal{A}_1, \dots, \mathcal{A}_s$ (from $\mathfrak{C}$) with back reference π, and $a_1, \dots, a_n \in S$, then

$$\begin{array}{rcl} \mathcal{S} & \models & \varphi[a_1, \dots, a_n] \\ \text{iff} \quad \mathcal{A}_1, \dots, \mathcal{A}_s & \models & \Delta[\pi(a_1), \dots, \pi(a_n)]. \end{array}$$

Intuitively, an $\oplus$-decomposition for a formula $\varphi(\overline{x})$ from $\mathsf{L}'[\sigma]$ on $\mathfrak{C}$ is a Boolean combination β of formulae from $\mathsf{L}[\sigma]$ which is equivalent to $\varphi(\overline{x})$ on any disjoint sum $\mathcal{S}$ of structures from $\mathfrak{C}$ when every formula in β is evaluated in one of the components of the disjoint sum. The sets $\Delta_1, \dots, \Delta_s$ determine in which component every formulae of β is evaluated in.

Example 5.1.5. In a graph, the $\mathsf{FO}[E]$-formula

$$\varphi(x) \;:=\; \exists y \exists z (\neg y{=}z \;\wedge\; \neg E(y,x) \;\wedge\; \neg E(z,x))$$

is satisfied if and only if there are at least two nodes that do not have an edge to x. Since every component of a disjoint sum has to be non-empty and there are no edges between nodes from different components, the reduction sequence

$$\big(X_{1,\psi} \;\vee\; X_{2,\psi} \vee (X_{1,\chi} \wedge X_{2,\delta}) \;\vee\; (X_{2,\chi} \wedge X_{1,\delta}), \{\psi, \chi, \delta\}, \{\psi, \chi, \delta\}\big)$$

with

$$\psi \;:=\; \exists y \neg E(y,x), \qquad \chi(x) \;:=\; x{=}x, \qquad \text{and} \qquad \delta \;:=\; \exists y \exists z \neg y{=}z$$

is a binary $\oplus$-decomposition for φ over $\mathsf{FO}[E]$ on the class of graphs.

5.2 Constructing Decompositions from Hanf Normal Form

Recall that $\mathfrak{C}^{d,\sigma}$, for $d \geq 0$, denotes the class of all d-bounded σ-structures. In this section, we present a worst-case optimal algorithm that computes, on input of a degree bound $d \geq 2$, a relational signature σ, an arity $s \geq 1$, and a formula from $\mathsf{FO}+\mathrm{un}\mathsf{M}[\sigma_s]$, an s-ary $\oplus$-decomposition over $\mathsf{FO}+\mathrm{un}\mathsf{M}[\sigma]$ on $\mathfrak{C}^{d,\sigma}$. The algorithm uses the construction of Hanf normal form from Theorem 3.2.1 in Chapter 3 and adds a second step which computes $\oplus$-decompositions for the sphere-formulae and counting-sentences of HNF-formulae on the class of all σ-structures.

Theorem 5.2.1. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *a relational signature σ,*
- *an arity $s \geq 1$,*
- *and a formula $\varphi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma_s]$ with $D \subseteq D_{\mathrm{all}}$, $n \coloneqq |\overline{x}|$ free variables, quantifier rank $q \geq 0$, and threshold $T \geq 0$,*

computes an s-ary $\oplus$-decomposition $(\beta, \Delta_1, \ldots, \Delta_s)$ for $\varphi(\overline{x})$ over $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma]$ on $\mathfrak{C}^{d,\sigma}$, where the sets $\Delta_1, \ldots, \Delta_s$ only contain HNF-formulae with threshold $< T + (n+q) \cdot \nu_d(4^q)$.

Furthermore, the algorithm computes Δ in time

$$(2\max\{1, T, P\})^{(||\varphi|| \cdot \nu_d(4^q))^{\mathcal{O}(||\sigma_s||)}},$$

where $P \geq 0$ is the maximum period of $\varphi(\overline{x})$.

Remark 5.2.2. Recall that $T, P, q < ||\varphi||$. If furthermore σ only contains the relation symbols that occur in $\varphi(\overline{x})$, also $||\sigma|| < ||\varphi||$. Under these assumptions, the algorithm takes 3-fold exponential time

$$2^{d^{s \cdot 2^{\mathcal{O}(||\varphi||)}}}$$

for $d = 3$, and, for $d = 2$, it takes 2-fold exponential time

$$2^{2^{s \cdot \mathrm{poly}(||\varphi||)}}.$$

For a degree bound $d \geq 2$, a relational signature σ, an arity $s \geq 1$, and a formula $\varphi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma_s]$, where $D \subseteq D_{\mathrm{all}}$, the proof of Theorem 5.2.1 proceeds in two main steps:

(Step 1) The algorithm of Theorem 3.2.1 turns the input formula $\varphi(\overline{x})$ into a d-equivalent HNF-formula $\psi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma_s]$.

(Step 2) Lemma 5.2.3 below replaces each counting-sentence and each sphere-formula in $\psi(\overline{x})$ by an s-ary $\oplus$-decomposition over $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma]$ on the class of all σ-structures.

Altogether, this yields an s-ary $\oplus$-decomposition for $\psi(\overline{x})$, and thus an s-ary $\oplus$-decomposition for $\varphi(\overline{x})$ on $\mathfrak{C}^{d,\sigma}$.

The following Lemma 5.2.3 provides the transformation of HNF-formulae into $\oplus$-decompositions. Note that the lemma is more general than actually needed for the proof of Theorem 5.2.1.

- The lemma constructs a $\oplus$-decomposition on the class of all σ-structures instead of just σ-structures of degree at most d.
- The lemma shows that for every HNF-formula from any logic $\mathsf{L}[\sigma_s]$ as defined in Section 2.4.2, there is a corresponding $\oplus$-decomposition over $\mathsf{L}[\sigma]$ on the class of all σ-structures. For an ultimately periodic logic L, the construction of Lemma 5.2.3 allows to be read as an algorithm. In particular, this holds for $\mathsf{FO}+\mathrm{un}\mathsf{M}$.

Lemma 5.2.3. *Let L be a logic, let σ be a relational signature, let $s \geq 1$, and let $\psi(\overline{x})$ be a HNF-formula from $\mathsf{L}[\sigma_s]$. There is an s-ary $\oplus$-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ for $\psi(\overline{x})$ over $\mathsf{L}[\sigma]$ on the class of all σ-structures, where all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF-formulae.*

Furthermore, if L is ultimately periodic, there is an algorithm which, on input of s and $\psi(\overline{x})$, computes Δ in time

$$s \cdot \mathcal{O}(||\psi||).$$

In particular, if $\psi(\overline{x})$ is from $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma_s]$ for some $D \subseteq D_{\mathrm{all}}$ and of threshold $T \geq 0$, then Δ is also over $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma]$, and all formulae in the sets $\Delta_1, \ldots, \Delta_s$ have threshold $\leq T$.

For the construction of s-ary $\oplus$-decompositions for counting-sentences and sphere-formulae, the following notation will be useful. We call a σ_s-structure $\mathcal{A}$ *monochrome (with colour i)* if there is an $i \in [1, s]$ such that $A = P_i^{\mathcal{A}}$ and $P_j^{\mathcal{A}} = \emptyset$

for all $j \in [1, s]$ with $j \neq i$. The crucial point in the proof of Lemma 5.2.3 is that in every σ_s-type $(\mathcal{B}, \overline{b})$ which can be realised by a tuple in a disjoint sum of of σ-structures $\mathcal{A}_1, \dots, \mathcal{A}_s$, the underlying σ_s-structure $\mathcal{B}$ is a union of pairwise disjoint monochrome σ_s-structures. This follows directly from the definition of disjoint sums.

Proof of Lemma 5.2.3. Let L be a logic, let σ be a relational signature, let $s \geq 1$, and let $\psi(\overline{x})$ be a HNF-formula from $\mathsf{L}[\sigma_s]$ with free variables from the tuple $\overline{x}$ of length $n \geq 0$.

The algorithm proceeds in the following steps:

(Step 1) Consider a counting-sentence $\chi = \mathsf{Q}y \ \mathrm{sph}_\tau(y)$ that occurs in $\psi(\overline{x})$ and recall that τ is a σ_s-type $(\mathcal{B}, b)$ with one centre.

(Case 1.a) If $\mathcal{B}$ is monochrome with colour $i \in [1, s]$, we replace χ in $\psi(\overline{x})$ by the propositional symbol $\beta^\chi := X_{i,\tilde{\chi}}$ and let

$$\tilde{\chi} \ := \ \mathsf{Q}y \ \mathrm{sph}_{\tilde{\tau}}(y),$$

where $\tilde{\tau} := (\mathcal{B}_{|\sigma}, b)$. Furthermore, we let $\Delta_i^\chi := \{\tilde{\chi}\}$ and $\Delta_j^\chi := \emptyset$ for all $j \in [1, s]$ with $j \neq i$.

(Case 1.b) If this is not the case, we replace χ in ψ by the Boolean constant

$$\beta^\chi \ := \ \begin{cases} \mathbf{1} & \text{if } 0 \in \mathsf{Q}, \quad \text{or} \\ \mathbf{0} & \text{if } 0 \notin \mathsf{Q}, \end{cases}$$

and let $\Delta_j^\chi := \emptyset$ for all $j \in [1, s]$.

We prove the following claim after completing the construction.

Claim 1. *$(\beta^\chi, \Delta_1^\chi, \dots, \Delta_s^\chi)$ is a $\oplus$-decomposition for χ.*

(Step 2) Consider a sphere-formula $\alpha(\overline{x}') = \mathrm{sph}_\varrho(\overline{x}')$ that occurs in $\psi(\overline{x})$. In particular, the tuple $\overline{x}'$ is of length $m \in [1, |\overline{x}|]$ and ϱ is a σ_s-type $(\mathcal{B}, \overline{b})$ with the m centres $\overline{b} = (b_1, \dots, b_m)$ and radius $r \geq 0$. We proceed as follows:

Choose $k \geq 1$ as the number of connected components which constitute the σ_s-structure $\mathcal{B}$, that is, the unique number k such that there are pairwise disjoint σ_s-structures $\mathcal{B}_1, \dots, \mathcal{B}_k$, each with a connected Gaifman graph, whose union is $\mathcal{B}$.

(Case 2.a) Suppose that each of the structures $\mathcal{B}_1, \dots, \mathcal{B}_k$ is monochrome. Let $J \subseteq [1, s]$ such that for each $j \in J$, there is at least one structure from $\mathcal{B}_1, \dots, \mathcal{B}_k$ with colour j. For each $j \in J$, let $j_m \in [1, m]$ and let $i_{j,1}, \dots, i_{j,j_m} \in [1, m]$ with $i_{j_1} < \cdots < i_{j,j_m}$ be the indices of all the elements from $b_1, \dots, b_m$ that belong to $P_j^{\mathcal{B}}$.

Moreover, let $\overline{b}_j := (b_{i_{j,1}}, \dots, b_{i_{j,j_m}})$ be the subtuple of $\overline{b}$ consisting of all these elements. Then, for each $j \in J$, the induced substructure $\mathcal{B}[N_r^{\mathcal{B}}(\overline{b}_j)]$ of $\mathcal{B}$ is the union of all structures $\mathcal{B}_i$ with $i \in [1, k]$ that are monochrome with colour j.

For each $j \in J$, we let $\tilde{\varrho}_j := (\mathcal{B}[N_r^{\mathcal{B}}(\overline{b}_j)_{|\sigma}, \overline{b}_j)$ and replace $\alpha(\overline{x}')$ by the propositional formula

$$\beta^\alpha \; := \; \bigwedge_{j \in J} X_{j, \alpha_j(\overline{x}'_j)}$$

where for each $j \in J$ we let $\overline{x}'_j := (x_{i_{j,1}}, \dots, x_{i_{j,j_m}})$ and $\alpha_j(\overline{x}'_j) := \mathrm{sph}_{\tilde{\varrho}_j}(\overline{x}'_j)$. Furthermore, we let $\Delta_j^\alpha := \{\alpha_j\}$ if $j \in J$ and, otherwise, $\Delta_j^\alpha := \emptyset$ for all $j \in [1, s]$.

(Case 2.b) Otherwise, that is, if at least one of the structures $\mathcal{B}_1, \dots, \mathcal{B}_k$ is not monochrome, we replace $\alpha(\overline{x}')$ with the Boolean constant $\beta^\alpha := \mathbf{0}$ and let $\Delta_j^\alpha := \emptyset$ for all $j \in [1, s]$.

We prove the following claim below.

Claim 2. *$(\beta^\alpha, \Delta_1^\alpha, \dots, \Delta_s^\alpha)$ is a $\oplus$-decomposition for $\alpha(\overline{x}')$.*

(Step 3) By β we denote the propositional formula obtained by replacing each counting-sentence χ and each sphere-formulae $\alpha(\overline{x})$ in $\psi(\overline{x})$ by the propositional formulae β^χ and β^α, respectively. . For each $i \in [1, s]$, we let Δ_i the union of the sets Δ_i^χ and Δ_i^α for all counting-sentences χ and all sphere-formulae α of $\psi(\overline{x})$.

Then, the s-ary reduction sequence $(\beta, \Delta_1, \dots, \Delta_s)$ is, according to Claim 1 and Claim 2, a $\oplus$-decomposition for $\psi(\overline{x})$.

By the construction just described it is clear that if $\psi(\overline{x})$ is from $\mathsf{L}[\sigma_s]$, then $\Delta_1, \dots, \Delta_s \subseteq \mathsf{L}[\sigma]$. In particular, if $\psi(\overline{x})$ is from $\mathsf{FO}{+}\mathrm{unM}[\sigma_s]$ and of threshold $T \geq 0$, all formulae in the sets $\Delta_1, \dots, \Delta_s$ are from $\mathsf{FO}{+}\mathrm{unM}[\sigma]$ and have threshold $\leq T$.

The proofs of Claim 1 and Claim 2 below are straightforward and use the notation introduced in the corresponding cases of the construction above. For both proofs, we let $\mathcal{S}$ be a disjoint sum of some arbitrary σ-structures $\mathcal{A}_1, \dots, \mathcal{A}_s$ with a back reference π. In particular, we suppose that the σ-reduct of $\mathcal{S}$ is the union of the pairwise disjoint σ-structures $\mathcal{A}'_1, \dots, \mathcal{A}'_s$ with $\mathcal{A}'_i \cong \mathcal{A}_i$ and $P_i^{\mathcal{S}} = A'_i$ for each $i \in [1, s]$.

Proof of Claim 1. We distinguish between Case (1.a) and Case (1.b) above.

If $\mathcal{B}$ is monochrome with a colour $i \in [1, s]$, the following equivalences hold:

$$\begin{array}{lll} & \mathcal{S} \models \chi & \\ \text{iff} & |\tau(\mathcal{S})| \in \mathsf{Q} & \\ \text{iff} & |\tilde{\tau}(\mathcal{A}'_i)| \in \mathsf{Q} & \text{(since } \mathcal{A}'_i \text{ is the } \sigma\text{-reduct of } \mathcal{S}[P_i^{\mathcal{S}}]) \\ \text{iff} & |\tilde{\tau}(\mathcal{A}_i)| \in \mathsf{Q} & \text{(since } \mathcal{A}'_i \cong \mathcal{A}_i) \\ \text{iff} & \mathcal{A}_i \models \tilde{\chi} & \\ \text{iff} & \mathcal{A}_1, \dots, \mathcal{A}_s \models \Delta^{\chi}. & \end{array}$$

If $\mathcal{B}$ is not monochrome, then $|\tau(\mathcal{S})| = 0$. Thus, the following equivalences hold:

$$\mathcal{S} \models \chi \quad \text{iff} \quad 0 \in \mathsf{Q} \quad \text{iff} \quad \mathcal{A}_1, \dots, \mathcal{A}_s \models \Delta^{\chi}.$$

This completes the proof of Claim 1.

Proof of Claim 2. Let $a_1, \dots, a_m \in S$. We distinguish between Case (2.a) and Case (2.b) above.

Suppose that each of the structures $\mathcal{B}_1, \dots, \mathcal{B}_k$ is monochrome. Furthermore, let $c_1, \dots, c_k \in [1, s]$ be the colours of the structures $\mathcal{B}_1, \dots, \mathcal{B}_k$. The following equivalences hold:

$$\begin{array}{lll} & \mathcal{S} \models \mathrm{sph}_{\varrho}[a_1, \dots, a_m] & \\ \text{iff} & \mathcal{N}_r^{\mathcal{S}}(a_{i_{j,1}}, \dots, a_{i_{j,j_m}}) \cong (\mathcal{B}[N_r^{\mathcal{B}}(\bar{b}_j)], \bar{b}_j) & \text{for all } j \in J \\ \text{iff} & \mathcal{N}_r^{\mathcal{A}'_{c_j}}(a_{i_{j,1}}, \dots, a_{i_{j,j_m}}) \cong \tilde{\varrho}_j & \text{for all } j \in J \\ \text{iff} & \mathcal{N}_r^{\mathcal{A}_{c_j}}(\pi(a_{i_{j,1}}), \dots, \pi(a_{i_{j,j_m}})) \cong \tilde{\varrho}_j & \text{for all } j \in J \\ \text{iff} & \mathcal{A}_{c_j} \models \alpha_j[\pi(a_{i_{j,1}}), \dots, \pi(a_{i_{j,j_m}})] & \text{for all } j \in J \\ \text{iff} & \mathcal{A}_1, \dots, \mathcal{A}_s \models \Delta^{\alpha}[\pi(a_1), \dots, \pi(a_m)]. & \end{array}$$

If one of the structures $\mathcal{B}_1, \dots, \mathcal{B}_k$ is not monochrome, then $\mathcal{S} \not\models \mathrm{sph}_{\varrho}[a_1, \dots, a_m]$ and, by construction, also $\mathcal{A}_1, \dots, \mathcal{A}_s \not\models \Delta^{\alpha}[\pi(a_1), \dots, \pi(a_m)]$.

This completes the proof of Claim 2.

Time complexity. In the following, we analyse the time required by the steps of the algorithm described above for the case of a HNF-formula from an ultimately periodic logic L.

(Step 1) Consider a counting-sentence $\chi = \mathsf{Q}y \ \mathrm{sph}_\tau(y)$ from $\psi(\overline{x})$ with a type $\tau = (\mathcal{B}, b)$. Recall that the sphere-formula sph_τ contains a conjunction of all (negated) atomic σ_s-formulae that hold for the elements of τ. Hence, by an examination of the sphere-formula sph_τ, it takes time in $\mathcal{O}(\chi)$ to decide whether $\mathcal{B}$ is monochrome and, if yes, to construct the counting-sentence $\tilde{\chi}$.

Since the sum of the length of the counting-sentences is bounded by the size of $\psi(\overline{x})$, Step (1) altogether needs time in $\mathcal{O}(||\psi||)$.

(Step 2) Consider a sphere-formula $\alpha(\overline{x}') = \mathrm{sph}_\varrho(\overline{x}')$ from $\psi(\overline{x})$ where $\varrho = (\mathcal{B}, \overline{b})$. Similar to the procedure in Step (1), it requires time in $\mathcal{O}(\alpha)$ to decide whether $\mathcal{B}$ is a union of pairwise disjoint monochrome σ_s-structures.

If this is the case, then for each $j \in J$, the same time is required to construct the sphere-formula $\alpha_j(\overline{x}'_j)$. For this, recall that the corresponding type ϱ_j contains precisely the j-coloured elements of ϱ.

Since $|J| \leq s$, the algorithm needs time in $s \cdot \mathcal{O}(\alpha)$ to compute the propositional formula for the sphere-formula $\alpha(\overline{x}')$.

As the sum of the lengths of the sphere-formulae is bounded by the size of $\psi(\overline{x})$, Step (2) altogether needs time in $s \cdot \mathcal{O}(||\psi||)$.

(Step 3) The size of the propositional formula β is in $s \cdot \mathcal{O}(||\psi||)$, which also bounds the time required to compute the sets $\Delta_1, \dots, \Delta_s$.

In summary, the construction of the reduction sequence $(\beta, \Delta_1, \dots, \Delta_s)$ on input of $\psi(\overline{x})$ takes time in $s \cdot \mathcal{O}(||\psi||)$. This completes the proof of Lemma 5.2.3. □

We are now ready to complete the proof of Theorem 5.2.1.

Proof of Theorem 5.2.1. We describe the algorithm on input of a degree bound $d \geq 2$, a relational signature σ, a number $s \geq 1$, and a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{unM}(D)[\sigma_s]$, for a set $D \subseteq D_{\mathrm{all}}$. Let $T, P, q \geq 0$ be the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$, respectively. Furthermore, let $n \coloneqq |\overline{x}|$ denote the number of free variables of $\varphi(\overline{x})$.

The algorithm proceeds as follows:

(Step 1) The algorithm of Theorem 3.2.1 constructs, on input of d, σ_s, and $\varphi(\overline{x})$, a HNF-formula $\psi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma_s]$ that is d-equivalent to $\varphi(\overline{x})$ and that has threshold $< T + (n+q) \cdot \nu_d(4^q)$. This takes time in

$$(2\max\{1, T, P\})^{(||\varphi|| \cdot \nu_d(4^q))^{\mathcal{O}(||\sigma_s||)}}. \qquad (1)$$

(Step 2) The algorithm of Lemma 5.2.3 computes, on input of the arity s and the HNF-formula $\psi(\overline{x})$, an s-ary $\oplus$-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ for $\psi(\overline{x})$ over $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma]$ on the class of all σ-structures. This requires time in $s \cdot \mathcal{O}(||\psi||)$. Since the size of $\psi(\overline{x})$ is bounded by the time required for its construction, this can also be bounded by Estimate (1).

Furthermore, by Lemma 5.2.3, all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF-formulae with threshold $\leq T$.

Since $\varphi(\overline{x})$ and $\psi(\overline{x})$ are d-equivalent, Δ is also an s-ary $\oplus$-decomposition for $\varphi(\overline{x})$ on $\mathfrak{C}^{d,\sigma}$. The overall time required by the algorithm to construct Δ can be bounded by Estimate (1). This completes the proof of Theorem 5.2.1. $\square$

5.3 Decompositions with respect to Transductions

In this section, we turn our attention from $\oplus$-decompositions to decompositions speaking about other forms of compositions of structures. More precisely, we show how to transfer the algorithm of Theorem 5.2.1 to an algorithm that produces decompositions on composite structures obtained by applying transductions to disjoint sums of structures. Note that, in [Mak04], transductions are used in a similar way to obtain the classical Feferman-Vaught theorem for so-called generalised products [FV59] from its special cases for disjoint unions and direct products of structures.

The following definition of such decompositions is more general than actually used in this section, but will be used in this general form later on in Section 7.4. Suppose that L and L' are logics.

Definition 5.3.1. Let σ and τ be relational signatures, and let $\mathfrak{C}$ be a class of σ-structures. Let $s \geq 1$ and let Θ be a transduction from σ_s to τ with arity $t \geq 1$. Let $\varphi(\overline{x})$ be a formula from $\mathsf{L}'[\tau]$, whose $n \geq 0$ free variables are given by the tuple $\overline{x} = (x_1, \ldots, x_n)$. For all $i \in [1, n]$, let furthermore $\overline{x}_i = (x_{i,1}, \ldots, x_{i,t})$.

A *Θ-decomposition for $\varphi(\overline{x})$ (on $\mathfrak{C}$) over* $\mathsf{L}[\sigma]$ is an s-ary reduction sequence $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ over $\mathsf{L}[\sigma]$, where the free variables of all formulae in the sets $\Delta_1, \ldots, \Delta_s$ all belong to the tuple $(\overline{x}_1, \ldots, \overline{x}_n)$, and for which the following holds:

If $\mathcal{S}$ is a disjoint sum of σ-structures $\mathcal{A}_1, \ldots, \mathcal{A}_s$ (from $\mathfrak{C}$) with back reference π, for which $\Theta[\mathcal{S}]$ is defined, and if $\overline{a}_i = (a_{i,1}, \ldots, a_{i,t})$ for each $i \in [1, n]$ belongs to the universe of $\Theta[\mathcal{S}]$, then

$$\begin{array}{rcl} \Theta[\mathcal{S}] & \models & \varphi[\overline{a}_1; \ldots; \overline{a}_n] \\ \text{iff} \quad \mathcal{A}_1, \ldots, \mathcal{A}_s & \models & \Delta[(\pi(a_{1,1}), \ldots, \pi(a_{1,t})), \ldots, (\pi(a_{n,1}), \ldots, \pi(a_{n,t}))]. \end{array}$$

The following lemma shows that a Θ-decomposition of an L'-formula φ can be obtained from a $\oplus$-decomposition of a Θ-reduct of φ from some logic L''.

Lemma 5.3.2. *Let $\mathsf{L}, \mathsf{L}', \mathsf{L}''$ be logics. Let σ and τ be relational signatures, and let $\mathfrak{C}$ be a class of σ-structures. Let $s \geq 1$ and let Θ be a transduction from σ_s to τ with arity $t \geq 1$.*

Suppose that φ is a formula from $\mathsf{L}'[\tau]$, that ψ is a Θ-reduct for φ from $\mathsf{L}''[\sigma_s]$, and that Δ is a t-ary $\oplus$-decomposition for ψ over $\mathsf{L}[\sigma]$ on $\mathfrak{C}$.

Then, Δ is a Θ-decomposition for φ over $\mathsf{L}[\sigma]$ on $\mathfrak{C}$.

Proof. The proof follows directly from the definitions. Let $\mathsf{L}, \mathsf{L}', \mathsf{L}''$ be logics. Let σ and τ be relational signatures, and let $\mathfrak{C}$ be a class of σ-structures. Let $s \geq 1$ and let Θ be a transduction from σ_s to τ with arity $t \geq 1$. Let $\varphi(\overline{x})$ be a formula from $\mathsf{L}'[\tau]$ with the $n \geq 0$ free variables $\overline{x} = (x_1, \ldots, x_n)$. For all $i \in [1, n]$, let furthermore $\overline{x}_i = (x_{i,1}, \ldots, x_{i,t})$.

Suppose that $\psi(\overline{x}_1, \ldots, \overline{x}_n)$ is a Θ-reduct for $\varphi(\overline{x})$ from $\mathsf{L}''[\sigma_s]$. Then, for every σ_s-structure $\mathcal{A}$ for which $\Theta[\mathcal{A}]$ is defined, and for all elements $\overline{a}_1, \ldots, \overline{a}_n$ from the universe of $\Theta[\mathcal{A}]$,

$$\begin{array}{rcl} \Theta[\mathcal{A}] & \models & \varphi[\overline{a}_1; \ldots; \overline{a}_n] \\ \text{iff} \quad \mathcal{A} & \models & \psi[\overline{a}_1, \ldots, \overline{a}_n]. \end{array} \tag{1}$$

Let Δ be a t-ary $\oplus$-decomposition for $\psi(\overline{x}_1, \ldots, \overline{x}_n)$ over $\mathsf{L}[\sigma]$ on $\mathfrak{C}$. If $\mathcal{S}$ is a disjoint sum with back reference π of σ-structures $\mathcal{A}_1, \ldots, \mathcal{A}_s \in \mathfrak{C}$ and if furthermore $\overline{a}_i = (a_{i,1}, \ldots, a_{i,t}) \in S^t$ for each $i \in [1, n]$, then

$$\begin{array}{rcl} \mathcal{S} & \models & \psi[\overline{a}_1, \ldots, \overline{a}_n] \\ \text{iff} \quad \mathcal{A}_1, \ldots, \mathcal{A}_s & \models & \Delta[(\pi(a_{1,1}), \ldots, \pi(a_{1,t})), \ldots, (\pi(a_{n,1}), \ldots, \pi(a_{n,t}))]. \end{array} \tag{2}$$

Hence, putting Equivalence (1) and Equivalence (2) together, we know that if $\mathcal{S}$ is a disjoint sum of σ-structures $\mathcal{A}_1, \ldots, \mathcal{A}_s \in \mathfrak{C}$ with back reference π, for which $\Theta[\mathcal{S}]$ is defined, and if $\overline{a}_i = (a_{i,1}, \ldots, a_{i,t}) \in S^t$ for each $i \in [1, n]$, then

$$\begin{array}{rcl} \Theta[\mathcal{S}] & \models & \varphi[\overline{a}_1; \ldots; \overline{a}_n] \\ \text{iff} \quad \mathcal{A}_1, \ldots, \mathcal{A}_s & \models & \Delta[(\pi(a_{1,1}), \ldots, \pi(a_{1,t})), \ldots, (\pi(a_{n,1}), \ldots, \pi(a_{n,t}))]. \end{array}$$

Thus, we can conclude that Δ is a Θ-decomposition for $\varphi(\overline{x})$ over $\mathsf{L}[\sigma]$ on $\mathfrak{C}$. $\square$

To actually compute Θ-decompositions on classes of structures of bounded degree, an algorithm first uses Lemma 2.6.4 to compute a reduct $\varphi^{-\Theta}$ of the input formula φ with respect to the transduction Θ, which is also given as an input to the algorithm. Afterwards, the algorithm of Theorem 5.2.1 is invoked on the reduct $\varphi^{-\Theta}$.

However, there is a catch. Suppose that Θ has arity $t \geq 2$, which is needed, e. g., for the construction of decompositions with respect to direct products of structures in the next Section 5.4. In this case, the construction of $\varphi^{-\Theta}$ may introduce tuple-counting quantifiers and thus, cannot serve as an input for Theorem 5.2.1 in general.

Therefore, in this and the next section, we restrict attention to input formulae from FO. Since a formula of the shape $\exists(y_1, \ldots, y_t)\, \psi$ can be replaced by the equivalent formula $\exists y_1 \cdots \exists y_t\, \psi$, Lemma 2.6.4 guarantees that, in this case, there is also a Θ-reduct for φ in FO.

In Chapter 7, we will see how to turn arbitrary formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ into equivalent formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$. This will allow us to extend the results of this section and the next to such formulae.

The main result of this section can now be stated as follows:

Theorem 5.3.3. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$,
- *relational signatures* σ *and* τ,
- *an arity* $s \geq 1$,
- *a transduction* Θ *from* σ_s *to* τ *with arity* $t \geq 1$ *and quantifier rank* $q_\Theta \geq 0$, *and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}[\tau]$ *with* $n := |\overline{x}|$ *free variables and quantifier rank* $q \geq 0$,

computes a Θ*-decomposition* $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ *over* $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ *for* $\varphi(\overline{x})$ *on* $\mathfrak{C}^{d,\sigma}$, *where all formulae in the sets* $\Delta_1, \ldots, \Delta_s$ *are* HNF*-formulae with threshold* $< (t \cdot (n+q) + q_\Theta) \cdot \nu_d(4^{t \cdot q + q_\Theta})$.

Furthermore, the algorithm computes Δ in time

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + 2^{\left(||\Theta|| \cdot ||\varphi|| \cdot \nu_d(4^{t \cdot q + q_\Theta})\right)^{\mathcal{O}(||\sigma_s||)}}$$

and of size

$$2^{\left(||\Theta|| \cdot ||\varphi|| \cdot \nu_d(4^{t \cdot q + q_\Theta})\right)^{\mathcal{O}(||\sigma_s||)}}.$$

Proof. Let $d \geq 2$ be a degree bound, let σ and τ be relational signatures, and let $s \geq 1$. Furthermore, let Θ be a transduction from σ_s to τ with arity $t \geq 1$ and quantifier rank $q_\Theta \geq 0$. Moreover, let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}[\tau]$ with quantifier rank $q \geq 0$, and the $n \geq 0$ free variables $\overline{x} = (x_1, \ldots, x_n)$. For all $i \in [1, n]$, let furthermore $\overline{x}_i = (x_{i,1}, \ldots, x_{i,t})$.

The algorithm proceeds in the two following steps:

(Step 1) The algorithm of Lemma 2.6.4 computes a Θ-reduct $\varphi^{-\Theta}(\overline{x}_1, \ldots, \overline{x}_n)$ for $\varphi(\overline{x})$ from $\mathsf{FO}_{\mathrm{tpl}}[\sigma_s]$ with quantifier rank $\leq t \cdot q + q_\Theta$, dimension $\leq t$, and $n \cdot t$ free variables. In particular, every quantified subformula of $\varphi^{-\Theta}$ is either of the shape $\exists y\, \varphi'$ or of the shape $\exists (y_1, \ldots, y_t)\, \varphi'$, where the latter can be replaced by a formula $\exists y_1 \cdots \exists y_t\, \varphi'$ to obtain a Θ-reduct $\psi(\overline{x}_1, \ldots, \overline{x}_n)$ for $\varphi(\overline{x})$ from $\mathsf{FO}[\sigma_s]$ which, in particular, has the same quantifier rank as $\varphi^{-\Theta}(\varphi)(\overline{x}_1, \ldots, \overline{x}_n)$.

(Step 2) Recall that each formula in $\mathsf{FO}[\sigma_s]$ has threshold 0. The algorithm of Theorem 5.2.1 is called on input of d, σ, s, and $\psi(\overline{x}_1, \ldots, \overline{x}_n)$, resulting in an s-ary $\oplus$-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ for $\psi(\overline{x}_1, \ldots, \overline{x}_n)$ over $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ on $\mathfrak{C}^{d,\sigma}$ where, in particular, all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF-formulae with threshold

$$< \ (t \cdot n + t \cdot q + q_\Theta) \cdot \nu_d(4^{t \cdot q + q_\Theta}) \ = \ (t \cdot (n + q) + q_\Theta) \cdot \nu_d(4^{t \cdot q + q_\Theta}).$$

By Lemma 5.3.2, we know that Δ is also a Θ-decomposition for $\varphi(\overline{x})$ over $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ on the class of d-bounded σ-structures.

Size and time complexity. We follow the steps of the algorithm.

(Step 1) The call of Lemma 2.6.4 on input of Θ and $\varphi(\overline{x})$ takes time in

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + ||\Theta|| \cdot \mathcal{O}(||\varphi||),$$

and yields a Θ-reduct $\varphi^{-\Theta}(\overline{x}_1, \ldots, \overline{x}_n)$ of size $||\Theta|| \cdot \mathcal{O}(||\varphi||)$. The construction of the $\mathsf{FO}[\sigma_s]$-formula $\psi(\overline{x}_1, \ldots, \overline{x}_n)$ from $\varphi^{-\Theta}(\overline{x}_1, \ldots, \overline{x}_n)$ takes time in $\mathcal{O}(||\varphi^{-\Theta}||)$.

(Step 2) By the upper bounds on the size and the quantifier rank of $\psi(\overline{x}_1, \dots, \overline{x}_n)$, the algorithm of Theorem 5.2.1 takes time in

$$2^{\left(||\Theta|| \cdot ||\varphi|| \cdot \nu_d(4^{t \cdot q + q_\Theta})\right)^{\mathcal{O}(||\sigma_s||)}}$$

to compute the Θ-decomposition Δ on input of d, σ, s, and $\psi(\overline{x}_1, \dots, \overline{x}_n)$. In particular, the latter estimate is also an upper bound on the size of Δ.

Altogether, the algorithm takes time in

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + 2^{\left(||\Theta|| \cdot ||\varphi|| \cdot \nu_d(4^{t \cdot q + q_\Theta})\right)^{\mathcal{O}(||\sigma_s||)}}$$

for the construction of Δ. This completes the proof of Theorem 5.3.3. □

5.4 Decompositions with respect to Direct Products

We conclude Chapter 5 with an exemplary application of Theorem 5.3.3 to direct products[2] (cf., e.g., [Hod93]). In the following, suppose that $\sigma = (R_1, \dots, R_\ell)$ is a relational signature with $\ell \geq 0$ relation symbols and let $s \geq 1$.

A σ-structure $\mathcal{P} = (P, R_1^{\mathcal{P}}, \dots, R_\ell^{\mathcal{P}})$ is the *direct product* of σ-structures $\mathcal{A}_1, \dots, \mathcal{A}_s$ if $P = A_1 \times \dots \times A_s$, and for each relation symbol R of arity $r \geq 1$ in σ, we have

$$R^{\mathcal{P}} \;\coloneqq\; \left\{ \begin{array}{ll} ((a_{1,1}, \dots, a_{1,s}), \dots, (a_{r,1}, \dots, a_{r,s})) \colon & (a_{1,i}, \dots, a_{r,i}) \in R^{\mathcal{A}_i} \\ & \text{for all } i \in [1, s] \end{array} \right\}.$$

We also denote the direct product of $\mathcal{A}_1, \dots, \mathcal{A}_s$ by $\mathcal{A}_1 \otimes \dots \otimes \mathcal{A}_s$. See Figure 5.1 for an example of a direct product. Analogous to $\oplus$-decompositions we define $\otimes$-decompositions. To this aim, we let L and L' be (not necessarily distinct) logics.

Definition 5.4.1. Let σ be a relational signature, let $\mathfrak{C}$ be a class of σ-structures, let $s \geq 1$, and let $\varphi(\overline{x})$ be a formula from $\mathsf{L}'[\sigma_s]$, whose $n \geq 0$ free variables are given by the tuple $\overline{x} = (x_1, \dots, x_n)$. For all $i \in [1, n]$ let furthermore $\overline{x}_i \coloneqq (x_{i,1}, \dots, x_{i,s})$.

An *s-ary $\otimes$-decomposition for $\varphi(\overline{x})$ (on $\mathfrak{C}$) over* $\mathsf{L}[\sigma]$ is an s-ary reduction sequence $\Delta = (\beta, \Delta_1, \dots, \Delta_s)$ over $\mathsf{L}[\sigma]$, where the free variables of the formulae

[2] also called tensor products or cartesian products

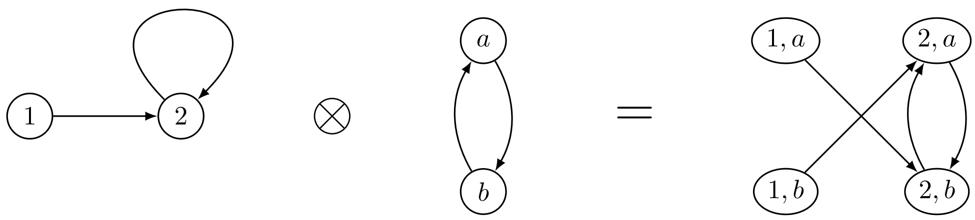

Figure 5.1 Example for the direct product of two (E)-structures with universe $\{1,2\}$ and universe $\{a,b\}$, respectively.

in the sets $\Delta_1, \ldots, \Delta_s$ belong to the tuple $(\overline{x}_1, \ldots, \overline{x}_n)$, and for which the following holds:

If $\mathcal{P}$ is the direct product of σ-structures $\mathcal{A}_1, \ldots, \mathcal{A}_s$ (from $\mathfrak{C}$) and if furthermore $\overline{a}_1, \ldots, \overline{a}_n \in P$, then

$$\begin{array}{rcl} \mathcal{P} & \models & \varphi[\overline{a}_1; \ldots; \overline{a}_n] \\ \text{iff} \quad \mathcal{A}_1, \ldots, \mathcal{A}_s & \models & \Delta[\overline{a}_1, \ldots, \overline{a}_n]. \end{array}$$

Direct products can be obtained from disjoint sums of σ-structures by transductions from σ_s to σ, which correspond to the definition of the universe and the relations of direct products [Mak04]. More precisely, we define for each $s \geq 1$ an s-ary transduction $\Theta_s^\sigma \coloneqq (\theta, \theta_{R_1}, \ldots, \theta_{R_\ell})$ with

$$\theta(x_1, \ldots, x_s) \ \coloneqq \ \bigwedge_{i=1}^{s} P_i(x_i)$$

and, for each relation symbol R of arity $r \geq 1$ from σ,

$$\theta_R(\overline{x}_1, \ldots, \overline{x}_r) \ \coloneqq \ \bigwedge_{i=1}^{s} R(x_{1,i}, \ldots, x_{r,i}),$$

where $\overline{x}_j \coloneqq (x_{j,1}, \ldots, x_{j,s})$ for each $j \in [1,r]$.

It is straightforward to verify that if $\mathcal{S}$ is a disjoint sum of σ-structures $\mathcal{A}_1, \ldots, \mathcal{A}_s$ with back reference π, and $\mathcal{P}$ is the direct product of $\mathcal{A}_1, \ldots, \mathcal{A}_s$, then

$$\Theta_s^\sigma[\mathcal{S}] \quad \cong \quad \mathcal{P}$$

by the isomorphism ϱ from $\Theta_s^\sigma[\mathcal{S}]$ to $\mathcal{P}$ defined by

$$\varrho(a_1, \ldots, a_s) \ = \ (\pi(a_1), \ldots, \pi(a_s)) \tag{5.1}$$

for all elements $(a_1, \ldots, a_s)$ in the universe of $\Theta_s^\sigma[\mathcal{S}]$.

The following lemma shows that the transductions just defined can indeed be used to obtain $\otimes$-decompositions.

Lemma 5.4.2. *Let* L *and* L' *be logics. Let* σ *be a relational signature and let* $\mathfrak{C}$ *be a class of* σ*-structures. Let* $s \geq 1$*, let* φ *be a formula from* $\mathsf{L}'[\sigma_s]$ *and suppose that* Δ *is a* Θ_s^σ*-decomposition for* φ *over* $\mathsf{L}[\sigma]$ *on* $\mathfrak{C}$*.*

Then, Δ *is also an* s*-ary* $\otimes$*-decomposition for* φ *over* $\mathsf{L}[\sigma]$ *on* $\mathfrak{C}$*.*

Proof. Let L and L' be logics. Let σ be a relational signature and let $\mathfrak{C}$ be a class of σ-structures. Let $s \geq 1$ and let $\varphi(\overline{x})$ be a formula from $\mathsf{L}'[\sigma_s]$ with the $n \geq 0$ free variables $\overline{x} = (x_1, \dots, x_n)$. Moreover, for all $i \in [1, n]$, let $\overline{x}_i = (x_{i,1}, \dots, x_{i,s})$.

Furthermore, let $\Delta = (\beta, \Delta_1, \dots, \Delta_s)$ be a Θ_s^σ-decomposition for $\varphi(\overline{x})$ over $\mathsf{L}[\sigma]$ on $\mathfrak{C}$. Recall that the free variables of all formulae in the sets $\Delta_1, \dots, \Delta_s$ belong to the tuple $(\overline{x}_1, \dots, \overline{x}_n)$.

If $\mathcal{S}$ is a disjoint sum with back reference π of σ-structures $\mathcal{A}_1, \dots, \mathcal{A}_s$ from $\mathfrak{C}$, ϱ is the isomorphism from $\Theta_s^\sigma[\mathcal{S}]$ to the direct product $\mathcal{P}$ of $\mathcal{A}_1, \dots, \mathcal{A}_s$ given by Equation (5.1), and $\overline{a}_i = (a_{i,1}, \dots, a_{i,s}) \in P$ for all $i \in [1, n]$, then the following equivalences hold:

$$\begin{array}{lrcl}
 & \mathcal{P} & \models & \varphi[\overline{a}_1; \dots; \overline{a}_n] \\
\text{iff} & \Theta_s^\sigma[\mathcal{S}] & \models & \varphi[\varrho^{-1}(\overline{a}_1); \dots; \varrho^{-1}(\overline{a}_n)] \\
\text{iff} & \Theta_s^\sigma[\mathcal{S}] & \models & \varphi[(\pi^{-1}(a_{1,1}), \dots, \pi^{-1}(a_{1,s})); \dots; (\pi^{-1}(a_{n,1}), \dots, \pi^{-1}(a_{n,s}))] \\
\text{iff} & \mathcal{A}_1, \dots, \mathcal{A}_s & \models & \Delta[(\pi(\pi^{-1}(a_{1,1})), \dots, \pi(\pi^{-1}(a_{1,s}))), \dots \\
 & & & \quad (\pi(\pi^{-1}(a_{n,1})), \dots, \pi(\pi^{-1}(a_{n,s})))] \\
\text{iff} & \mathcal{A}_1, \dots, \mathcal{A}_s & \models & \Delta[\overline{a}_1, \dots, \overline{a}_n].
\end{array}$$

Hence, we can conclude that Δ is an s-ary $\otimes$-decomposition for $\varphi(\overline{x})$ over $\mathsf{L}[\sigma]$ on $\mathfrak{C}$. □

This leads to the following application of Theorem 5.3.3.

Theorem 5.4.3. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$*,*
- *a relational signature* σ*,*
- *an arity* $s \geq 1$*, and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}[\sigma_s]$ *with* $n := |\overline{x}|$ *free variables and quantifier rank* $q \geq 0$*,*

computes an s-ary $\otimes$-decomposition $(\beta, \Delta_1, \ldots, \Delta_s)$ for $\varphi(\overline{x})$ over $\mathsf{FO}{+}\mathrm{unT}[\sigma]$ *on the class of d-bounded σ-structures, where all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are* HNF*-formulae with threshold $< s \cdot (n+q) \cdot \nu_d(4^{s \cdot q})$.*

Furthermore, the algorithm computes Δ in time

$$2^{\left(||\varphi|| \cdot \nu_d(4^{s \cdot q})\right)^{\mathcal{O}(||\sigma_s|| \cdot \log ||\sigma_s||)}}.$$

Proof of Theorem 5.4.3. Let $d \geq 2$ be a degree bound, let σ be a relational signature, let $s \geq 1$, and let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}[\sigma]$ with $n := |\overline{x}|$ free variables and quantifier rank $q \geq 0$.

On input of d, the signatures σ_s and σ, the transduction Θ_s^σ defined above, and the formula $\varphi(\overline{x})$, the algorithm of Theorem 5.3.3 computes a Θ_s^σ-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ over $\mathsf{FO}{+}\mathrm{unT}[\sigma]$ for $\varphi(\overline{x})$ on the class of all d-bounded σ-structures where, in particular, all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF-formulae with threshold $< s \cdot (n+q) \cdot \nu_d(4^{s \cdot q})$.

By Lemma 5.4.2, we know that Δ is also a $\otimes$-decomposition for $\varphi(\overline{x})$ over $\mathsf{FO}{+}\mathrm{unT}[\sigma]$ on the class of d-bounded σ-structures.

Time complexity. Clearly, the transduction Θ_s^σ is of quantifier rank 0 and can be computed in time $s \cdot \mathcal{O}(||\sigma||)$. Therefore, the call of the algorithm of Theorem 5.3.3 needs time in

$$s \cdot \mathcal{O}(||\sigma||)^2 + 2^{\left(s \cdot \mathcal{O}(||\sigma||) \cdot ||\varphi|| \cdot \nu_d(4^{s \cdot q})\right)^{\mathcal{O}(||\sigma_s||)}} \quad \subseteq \quad 2^{\left(||\varphi|| \cdot \nu_d(4^{s \cdot q})\right)^{\mathcal{O}(||\sigma_s|| \cdot \log ||\sigma_s||)}}.$$

This completes the proof of Theorem 5.4.3. $\square$

5.5 Conclusion

In this chapter, we have shown how to compute $\oplus$-decompositions for formulae from $\mathsf{FO}{+}\mathsf{unM}$ on classes of d-bounded structures. For $d \geq 3$, the corresponding algorithm has 3-fold exponential running time in the size of the formula to be decomposed. For $d = 2$, its running time is 2-fold exponential. In Section 9.5, we will provide matching lower bounds, showing that, for both cases, this algorithm is worst-case optimal.

In a first step, the algorithm relies on the construction of Hanf normal form, presented in Chapter 3. Its second step is a construction of $\oplus$-decompositions for the individual counting-sentences and sphere-formulae of the Hanf normal form. The restriction to degree-bounded structures is only required for the construction of Hanf normal form, while the second step is irrespective of the degree bound.

In the remainder of the chapter, we have extended this algorithm to decompositions defined by transductions on disjoint sums. In particular, this includes direct products. Due to the fact that the construction of reducts with respect to a transduction of arity ≥ 2 may introduce tuple-counting quantifiers, we restricted ourselves here to the case of input formulae from FO, where tuple-quantifiers can easily be resolved. The obtained algorithms have roughly the same running time as the algorithm for $\oplus$-decompositions.

In Section 7.4, the handling of tuple-counting quantifiers, described there, will allow us to extend all the above mentioned algorithms to input formulae from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$. Finally, Section 8.5 generalises these algorithms further to all ultimately periodic logics. There, we will also show that only for ultimately periodic logics $\oplus$-decompositions for the formulae of the logic are guaranteed to exist.

6 Preservation Theorems

It is known that, for FO-sentences that are preserved under extensions on a certain class of acyclic structures of unbounded degree, equivalent existential sentences can grow non-elementarily [DGKS07]. Similar non-elementary lower bounds also hold in respect to existential-positive sentences for FO-sentences that are preserved under homomorphisms [Ros08].

This chapter investigates algorithmic versions of preservation theorems on classes of structures of bounded degree. The results of this chapter are based on [HHS14, HHS15]. Its first result is an elementary algorithm which, on input of an $\mathsf{FO}+\mathrm{un}\mathsf{M}$-formula that is preserved under extensions on the class of d-bounded structures, computes a d-equivalent existential formula. For $d \geq 3$, the algorithm takes 5-fold exponential time in the size of the input formula.

A second result is an elementary algorithm which, on input of a formula from $\mathsf{FO}+\mathrm{un}\mathsf{M}$ that is preserved under homomorphisms on the class of d-bounded structures, computes a d-equivalent existential-positive formula. For $d \geq 3$, this algorithm takes 4-fold exponential time.

6.1 Introduction

Before stating the two main results of this chapter, we explain what it means for a formulae to be preserved under extensions or preserved under homomorphisms on a class of structures. Furthermore, we introduce the corresponding normal forms, called existential and existential-positive formulae (cf., e.g, [Hod93, Lyn59, Ros08]).

Throughout this chapter, σ will always denote a relational signature. Furthermore, in the following definitions, we let $\mathfrak{C}$ denote a class of σ-structures, and we let L denote one of the logics defined in Section 2.4.2

A σ-structure $\mathcal{B}$ is an *extension* of a σ-structure $\mathcal{A}$ if $\mathcal{A}$ is an *induced* substructure of $\mathcal{B}$.

Definition 6.1.1. A formula $\varphi(\overline{x})$ from $\mathsf{L}[\sigma]$ is *preserved under extensions on* $\mathfrak{C}$ if the following holds for each interpretation $(\mathcal{A}, \overline{a})$ for $\varphi(\overline{x})$ with $\mathcal{A} \in \mathfrak{C}$:

$$\text{if} \quad \mathcal{A} \models \varphi[\overline{a}] \quad \text{then} \quad \mathcal{B} \models \varphi[\overline{a}] \quad \text{for each extension } \mathcal{B} \in \mathfrak{C} \text{ of } \mathcal{A}.$$

Definition 6.1.2. A formula from $\mathsf{FO}[\sigma]$ is *existential* if it has the shape

$$\exists x_1 \cdots \exists x_n \, \varphi(x_1, \ldots, x_n)$$

where φ is quantifier-free.

It is straightforward to see that every existential $\mathsf{FO}[\sigma]$-formula is preserved under extensions on arbitrary classes of σ-structures.

Example 6.1.3. The $\mathsf{FO}[E]$-sentence

$$\varphi \;:=\; \exists x \exists y \exists z \Big(\neg x{=}y \;\wedge\; \neg y{=}z \;\wedge\; \neg z{=}x \;\wedge\; E(x,y) \;\wedge\; E(y,z) \;\wedge\; E(z,x) \Big)$$

states in a graph that there are three distinct nodes which form a triangle. As the sentence is existential, we know that it is preserved under extensions on all graphs.

Recall that a *homomorphism* from a σ-structure $\mathcal{A}$ to a σ-structure $\mathcal{B}$ is a mapping $h\colon A \to B$ such that for each relation symbol R of arity $r \geq 1$ from σ and all tuples $(a_1, \ldots, a_r) \in A^r$, if $(a_1, \ldots, a_r) \in R^{\mathcal{A}}$ then $(h(a_1), \ldots, h(a_r)) \in R^{\mathcal{B}}$. If $\overline{a} = (a_1, \ldots, a_n) \in A^n$ for an $n \geq 0$, we also write in the following $h(\overline{a})$ for the tuple $(h(a_1), \ldots, h(a_n))$, that is, we apply the homomorphism h component-wise to the tuple $\overline{a}$.

Definition 6.1.4. A formula $\varphi(\overline{x})$ from $\mathsf{L}[\sigma]$ with a tuple $\overline{x}$ of $n \geq 0$ variables is *preserved under homomorphisms on* $\mathfrak{C}$ if the following holds for each interpretation $(\mathcal{A}, \overline{a})$ for $\varphi(\overline{x})$ with $\mathcal{A} \in \mathfrak{C}$ and $\overline{a} \in A^n$:

$$\begin{aligned} \text{if} \quad & \mathcal{A} \models \varphi[\overline{a}] \\ \text{then} \quad & \mathcal{B} \models \varphi[h(\overline{a})] \quad \text{for every } \sigma\text{-structure } \mathcal{B} \in \mathfrak{C} \text{ for which} \\ & \text{there is a homomorphism } h \text{ from } \mathcal{A} \text{ to } \mathcal{B}. \end{aligned}$$

Definition 6.1.5. An *existential-positive* formula from $\mathsf{FO}[\sigma]$ is an existential formula that does not contain the symbol $\neg$ (and thus, also not the abbreviations $\to$ and $\leftrightarrow$). Furthermore, also the symbol $\perp$ is understood as an existential-positive formula that is not satisfied by any σ-structure.

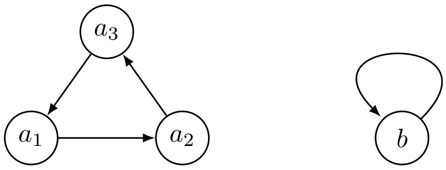

Figure 6.1 Two graphs $\mathcal{A}$ and $\mathcal{B}$ with a homomorphism from $\mathcal{A}$ to $\mathcal{B}$.

The symbol $\perp$ is introduced since every formula $\varphi(\overline{x})$ that is not satisfied by any interpretation $(\mathcal{A}, \overline{a})$ with $\mathcal{A} \in \mathfrak{C}$ is preserved under homomorphisms, but there is no unsatisfiable existential formula that does not makes use of negations.

Again, it is straightforward to see that every existential-positive $\mathsf{FO}[\sigma]$-formula is preserved under homomorphisms on arbitrary classes of σ-structures.

Example 6.1.6. The sentence $\mathsf{FO}[E]$-sentence φ from Example 6.1.3 is existential, but not existential-positive. It is also straightforward to see that it is not preserved under homomorphisms on the class of graphs. For example, the graph $\mathcal{A}$ consisting of three nodes a_1, a_2, and a_3 and edges from a_1 to a_2, a_2 to a_3, and a_3 to a_1 is a model of φ. On the other hand, the graph $\mathcal{B}$ consisting of one node b with an edge to itself is not a model of φ. However, the function that maps each of the nodes a_1, a_2, a_3 to b is a homomorphism from $\mathcal{A}$ to $\mathcal{B}$ (see also Figure 6.1).

In the following, we explore the complexity of constructing existential (respectively, existential-positive) formulae for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$ that are preserved under extensions (respectively, homomorphisms) on classes of degree bounded σ-structures that are closed under disjoint unions and closed under induced substructures (respectively, closed under disjoint unions, closed under induced substructures, and decidable in 1-fold exponential time).

It is straightforward to see that, e. g., the class $\mathfrak{C}^{d,\sigma}$ of all finite σ-structures of degree at most d, for any fixed $d \geq 0$, meets all these requirements.

The precise statements of this chapters first main result reads as follows; a proof is given in Section 6.2.

Theorem 6.1.7. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$*,*
- *a relational signature* σ*, and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$*,*

constructs an existential formula $\psi(\overline{x})$ *from* $\mathsf{FO}[\sigma]$ *such that the following holds for any class* $\mathfrak{D}$ *of* d*-bounded* σ*-structures that is closed under disjoint unions and induced substructures: If* $\varphi(\overline{x})$ *is preserved under extensions on* $\mathfrak{D}$*, then* $\varphi(\overline{x})$ *and* $\psi(\overline{x})$ *are* $\mathfrak{D}$*-equivalent.*

Furthermore, the algorithm computes $\psi(\overline{x})$ *in time*

$$||\varphi|| \cdot \left(2^{\nu_d(2^{\nu_d(4^q)^{\mathcal{O}(||\sigma||)}})} \cdot (T+n+q) \cdot L\right)^{(n+q)\cdot\mathcal{O}(\log\max\{1,T,P\})},$$

where $T, P, n, q \geq 0$ *and* $L \geq 1$ *are the threshold, the maximum period, the number of free variables, the quantifier rank, and the least common multiple of the periods of all modulo-counting quantifiers in* $\varphi(\overline{x})$*, respectively. In particular, the constants suppressed by the* $\mathcal{O}$*-notation do not depend on the signature* σ*.*

For the case of input sentences from $\mathsf{FO}+\mathrm{unM}(\{\mathsf{D}_p\})$ with threshold 0, where D_p is a single modulo-counting quantifier with period $p \geq 2$, Theorem 6.1.7 was already proven in [HHS14, HHS15].

Remark 6.1.8. Suppose that σ only contains relation symbols that actually occur in $\varphi(\overline{x})$ and thus, $||\sigma|| < ||\varphi||$. We know that $T, P, n, q < ||\varphi||$. Moreover, $L = 1$ if there are no modulo-counting quantifiers in φ, and otherwise

$$L \;\leq\; P! \;\leq\; 2^{P\cdot\log P}.$$

Thus, for every degree bound $d \geq 3$, the algorithm of Theorem 6.1.7 takes 5-fold exponential time in the size of the input formula $\varphi(\overline{x})$, that is, time in

$$2^{d^{2^{d^{2^{\mathcal{O}(||\varphi||)}}}}},$$

and for $d = 2$, the algorithm takes 3-fold exponential time, that is, time in

$$2^{2^{2^{\mathrm{poly}(||\varphi||)}}}.$$

In Section 9.6, this is complemented by a 3-fold exponential lower bound.

Remark 6.1.9. Moreover, for input sentences φ from FO, that is, for formulae where $T = P = n = 0$ and $L = 1$, the running time of the algorithm of Theorem 6.1.7 can be bounded by the simpler expression

$$||\varphi|| \cdot 2^{\nu_d(2^{\nu_d(4^q)^{\mathcal{O}(||\sigma||)}})}.$$

This chapters second main result reads as follows; a proof is given in Section 6.3 below. Here, we say that a class $\mathfrak{C}'$ of structures is decidable in time $t(n)$ for some function $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$ if there is an algorithm which decides on input of a signature σ and a σ-structure $\mathcal{A}$ in time $t(||\sigma|| + ||\mathcal{A}||)$ whether $\mathcal{A} \in \mathfrak{C}'$. Note that here, the class $\mathfrak{C}'$ is not restricted to structures over a specific signature (which is provided as input to the algorithm).

Theorem 6.1.10. *Let $\mathfrak{C}'$ a class of structures that is decidable in time $t(n)$ for some function $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$ and that is closed under disjoint unions and induced substructures.*

There is an algorithm which, on input of

- *a degree bound $d \geq 2$,*
- *a relational signature σ, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$,*

constructs an existential-positive formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ such that the following holds for the class $\mathfrak{D}$ of d-bounded σ-structures from $\mathfrak{C}'$: If $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, then $\varphi(\overline{x})$ and $\psi(\overline{x})$ are $\mathfrak{D}$-equivalent.

Furthermore, the algorithm computes $\psi(\overline{x})$ in time

$$2^{||\varphi||\cdot(n+1)^{\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}} \cdot t\big((n+1)^{\mathcal{O}(||\sigma||)} \cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}\big)$$

where $n, q \geq 0$ are the number of free variables and the quantifier rank of $\varphi(\overline{x})$, respectively. Moreover, the formula $\psi(\overline{x})$ is of size

$$2^{(n+1)^{\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}}.$$

For the case of input sentences from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(\{\mathsf{D}_p\})$ with threshold 0, where D_p is a single modulo-counting quantifier with period $p \geq 2$, Theorem 6.1.10 was already proven in [HHS14, HHS15].

Remark 6.1.11. Note that, in contrast to Theorem 6.1.7, the running time of the algorithm neither depends on the threshold nor on the periods of the modulo-counting quantifiers in the input formula.

Suppose that the function $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$ is at most 1-fold exponential (this is clearly the case if, e.g., $\mathfrak{C}'$ is the class of all structures). Recall that $n, q < ||\varphi||$. If we suppose that σ contains only the relation symbols that actually occur in $\varphi(\overline{x})$, that is, $||\sigma|| < ||\varphi||$ then, for every degree bound $d \geq 3$, the algorithm of

Theorem 6.1.10 takes 4-fold exponential time in the size of the input formula $\varphi(\overline{x})$, that is, time in

$$2^{2^{d^{2^{\mathcal{O}(||\varphi||)}}}}$$

and the size of $\psi(\overline{x})$ is bounded by the same expression.

For degree bound $d = 2$, the algorithm takes 3-fold exponential time

$$2^{2^{2^{\mathrm{poly}(||\varphi||}}}$$

and the size of $\psi(\overline{x})$ is again bounded by the same expression.

In Section 9.6, this is complemented by a 3-fold exponential lower bound.

Remark 6.1.12. For input sentences φ from FO, that is, for formulae where $n = 0$, the running time of the algorithm of Theorem 6.1.10 can be bounded by

$$2^{||\varphi||\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}} \cdot t(2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}),$$

and the size of the computed existential-positive sentence ψ by

$$2^{2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}}.$$

In Section 6.4, we present two examples of classes of structures, which show that the closure properties required in Theorem 6.1.7 and Theorem 6.1.10 are indeed necessary, and not just an artifact of the specific proofs.

A key concept in the proofs of Theorem 6.1.7 and Theorem 6.1.10 are minimal models of formulae. Again, we denote by $\mathfrak{C}$ a class of σ-structures.

Definition 6.1.13. Let $\varphi(\overline{x})$ be a formula from $\mathsf{L}[\sigma]$. An interpretation $(\mathcal{A}, \overline{a})$ for $\varphi(\overline{x})$ with $\mathcal{A} \in \mathfrak{C}$ is called a $\mathfrak{C}$*-minimal model of* φ if $\mathcal{A} \models \varphi[\overline{a}]$, but $\mathcal{B} \not\models \varphi[\overline{a}]$ for every proper induced substructure $\mathcal{B}$ of $\mathcal{A}$ that belongs to $\mathfrak{C}$ and that contains all the elements from the tuple $\overline{a}$.

Let $d \geq 0$ and let $\mathfrak{D}$ be a class of d-bounded σ-structures that is closed under disjoint unions and closed under induced substructures. The main combinatorial parts (Theorem 6.2.1 and Theorem 6.3.1) of the proofs of Theorem 6.1.7 and Theorem 6.1.10 provide upper bounds on the size of the universe of $\mathfrak{D}$-minimal models for formulae from $\mathsf{FO}{+}\mathrm{unM}[\sigma]$ that are preserved under extensions (respectively, homomorphisms) on $\mathfrak{D}$.

The proofs of both upper bounds on the size of the universe of $\mathfrak{D}$-minimal models proceed as follows: Suppose that $\varphi(\overline{x})$ is a formula from $\mathsf{FO}{+}\mathrm{unM}[\sigma]$

that is preserved under extensions (homomorphisms) on $\mathfrak{D}$. For a contradiction, we assume that there is a $\mathfrak{D}$-minimal model $(\mathcal{A}, \overline{a})$ of $\varphi(\overline{x})$ where the cardinality of A exceeds the upper bound. Then, a proper induced substructure $\mathcal{A}' \in \mathfrak{D}$ of $\mathcal{A}$ can be constructed such that $(\mathcal{A}', \overline{a})$ is also a model of $\varphi(\overline{x})$. This is a contradiction to the minimality of $(\mathcal{A}, \overline{a})$.

In both cases, we use the variant of Nurmonen's theorem [Nur00], stated in Theorem 3.3.1, which provides us with local conditions that make two interpretations indistinguishable for $\varphi(\overline{x})$.

The proof of Theorem 6.1.7 employs a novel inductive construction that constructs a sequence $(\mathcal{C}_i)_{i\geq 0}$ of structures from $\mathfrak{D}$ that alternates between proper induced substructures and disjoint extensions of $\mathcal{A}$ and finally stops with two consecutive structures $\mathcal{C}_i$ and $\mathcal{C}_{i+1}$ for some $i \geq 0$ such that the interpretations $(\mathcal{C}_i, \overline{a})$ and $(\mathcal{C}_{i+1}, \overline{a})$ can not be distinguished by $\varphi(\overline{x})$.

The proof of Theorem 6.1.10 is an adaptation of a result by Ajtai and Gurevich (Lemma 7.1 in [AG94]) where we use Theorem 3.3.1 instead of Gaifman's theorem.

Recall that an r-scattered set of elements in a structure $\mathcal{A}$, for some $r \geq 0$, is a set of elements of pairwise distance $> r$ in $\mathcal{A}$. Both proofs for lower bounds on the size of $\mathfrak{D}$-minimal models make use of the following easy fact.

Lemma 6.1.14 (cf., e.g., [ADG08])**.** *Let $d \geq 0$ be a degree bound and let $\mathcal{A}$ be a d-bounded σ-structure. For all $m, r \geq 0$, the following holds: If*

$$|A| \;>\; (m{-}1) \cdot \nu_d(2r),$$

then there exists an r-scattered subset of A with cardinality m.

Proof. Let $d \geq 0$ be a degree bound and let $\mathcal{A}$ be a d-bounded σ-structure. For $m, r \geq 0$, we show that if there is no r-scattered subset of A with cardinality m, then $|A| \leq (m{-}1) \cdot \nu_d(2r)$.

Choose a number $n < m$ such that there is an r-scattered set $B \subseteq A$ with cardinality n in $\mathcal{A}$, but no r-scattered subset of cardinality greater than n. Every element a of A has to be contained in the $2r$-neighbourhood of B (for otherwise, $B \cup \{a\}$ would be an r-scattered subset of A with cardinality $n + 1$). Therefore,

$$|A| \;=\; |N_{2r}^{\mathcal{A}}(B)| \;\leq\; (m{-}1) \cdot \nu_d(2r). \qquad \square$$

Finally, the upper bounds on the size of the universe of $\mathfrak{D}$-minimal models are used as an input to algorithms that compute a $\mathfrak{D}$-equivalent existential (existential-positive) $\mathsf{FO}[\sigma]$-formula for the input formula $\varphi(\overline{x})$.

The construction for existential formulae for formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}[\sigma]$ generalises Lemma 8.4 in [DGKS07]. Here, the handling of modulo-counting quantifiers uses the divide-and-conquer approach described in Section 2.9 to ensure the desired time complexity.

The construction for existential-positive sentences uses an algorithmic version of the Chandra-Merlin theorem ([CM77], cf., e.g., [AHV95]), which requires an additional assumption on the decidability of $\mathfrak{D}$.

Recall that for all $d \geq 0$ and $r \geq 0$, $\mathfrak{T}_r^{d,\sigma}(1)$ is the set of all (up to isomorphism) one-centred types with radius r that may be realised in a d-bounded σ-structure. For the rest of this chapter, we abbreviate

$$S^{d,s}(r) \;\; := \;\; 2^{\nu_d(r)^{\mathcal{O}(s)}}.$$

That is, $S^{\cdot,\cdot}(\cdot)$ is the set of all functions $f\colon \mathbb{N} \times \mathbb{N} \times \mathbb{N}_{\geq 1} \to \mathbb{N}$ where there is a number $c \in \mathbb{N}_{\geq 1}$ such that

$$f(d,r,s) \;\leq\; 2^{\nu_d(r)^{c \cdot s}}$$

for all $d, r \geq 0$ and $s \geq 1$. Note that, in particular, there is a function $f \in S$ such that for all $d \geq 2$ and $r \geq 1$ we have $|\mathfrak{T}_r^{d,\sigma}(1)| \leq f(d,r,||\sigma||)$.

6.2 Preservation under Extensions

This section is devoted to the proof of Theorem 6.1.7. In the following, we let $d \geq 2$ a degree bound and denote by $\mathfrak{D}$ a class of d-bounded σ-structures that is closed under disjoint unions and induced substructures.

The main combinatorial contribution of this section is an upper bound on the size of $\mathfrak{D}$-minimal models for formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}[\sigma]$ that are preserved under extensions on $\mathfrak{D}$, which is provided by Theorem 6.2.1 below. Afterwards, Lemma 6.2.2 uses this upper bound to construct existential formulae. The section concludes with the actual proof of Theorem 6.1.7, which combines the aforementioned steps.

Theorem 6.2.1. *There is a function $N\colon \mathbb{N}^6 \to \mathbb{N}$ with*

$$N^{d,||\sigma||}(T,n,q,L) \quad \in \quad S^{d,||\sigma||}(S^{d,||\sigma||}(4^q)) \cdot (T{+}n{+}q) \cdot L,$$

such that the following holds for every relational signature σ, every degree bound $d \geq 2$, every class $\mathfrak{D}$ of d-bounded σ-structures that is closed under disjoint unions and induced substructures, and every formula $\varphi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{M}[\sigma]$:

If $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{D}$, then every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of size at most $N^{d,||\sigma||}(T,n,q,L)$, where $T,n,q \geq 0$ are the threshold, the number of free variables, and the quantifier rank of $\varphi(\overline{x})$, and where $L \geq 1$ is the least common multiple of the periods of all modulo-counting quantifiers that appear in $\varphi(\overline{x})$.

Proof. Let σ be a relational signature, let $d \geq 2$, and let $\mathfrak{D}$ be a class of d-bounded σ-structures that is closed under disjoint unions and induced substructures.

Furthermore, let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}+\mathrm{un}\mathsf{M}[\sigma]$ that is preserved under extensions on $\mathfrak{D}$. Let T, $q \geq 0$ be the threshold and the quantifier rank of φ, let $n := |\overline{x}|$ be the number of free variables of $\varphi(\overline{x})$, and let $L \geq 1$ be the least common multiple of the periods of all modulo-counting quantifiers that appear in $\varphi(\overline{x})$.

Choose $r := 4^q$ and the threshold

$$t \;:=\; T + (n{+}q) \cdot \nu_d(r) \tag{1}$$

from Condition (3) of Theorem 3.3.1 for the numbers T, n, q, and r.

Furthermore, let

$$s \;\in\; S^{d,||\sigma||}(r)$$

be the number of non-isomorphic σ-types with radius r and one centre that may be realised in structures from $\mathfrak{D}$ and let

$$R \;:=\; 2s \cdot r, \quad \text{and} \quad S \;\in\; S^{d,||\sigma||}(R)$$

be the number of non-isomorphic σ-types with radius R and one centre that may be realised in σ-structures from $\mathfrak{D}$.

Towards a contradiction, assume that $\varphi(\overline{x})$ has a $\mathfrak{D}$-minimal model $(\mathcal{A}, \overline{a})$ with a universe of size

$$|A| \;>\; (2S \cdot t \cdot L + n - 1) \cdot \nu_d(2R).$$

By Lemma 6.1.14, there exists an R-scattered subset Z of A of cardinality $2S \cdot t \cdot L + n$. Suppose that $\overline{a} = (a_1, \ldots, a_n)$ and observe that

- each of the elements a_i with $i \in [1,n]$ only belongs to the R-neighbourhood of at most one element of Z, and that
- there are at most S pairwise non-isomorphic σ-type with radius R and one centre realised in $\mathcal{A}$.

Then, there is an R-scattered set $Y \subseteq Z$ with cardinality $2t \cdot L$, whose elements all realise the same type from $\mathfrak{T}_r^{d,\sigma}(1)$ and such that none of the elements a_i with $i \in [1,n]$ belong to the R-neighbourhood of Y.

In the following, we call a type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$ *frequent in a structure* $\mathcal{A}$ if $|\tau(\mathcal{A})| \geq t$. Otherwise, it is *rare in* $\mathcal{A}$. Note that each type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$ that is realised by an element from the $(R{-}r)$-neighbourhood of Y is frequent in $\mathcal{A}$, because it occurs at least $2t \cdot L \geq t$ times in $\mathcal{A}$.

Let X be a subset of Y with cardinality $t \cdot L$. Since

$$\mathcal{N}_R^{\mathcal{A}}(a) \;\cong\; \mathcal{N}_R^{\mathcal{A}}(b) \quad \text{for each } a \in X \text{ and each } b \in Y \setminus X, \tag{2}$$

the following holds for each type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$:

$$\text{If} \quad |\tau(\mathcal{A}) \cap N_{R-r}^{\mathcal{A}}(X)| \;\geq\; t, \quad \text{also} \quad |\tau(\mathcal{A} - N_{R-r}^{\mathcal{A}}(X))| \;\geq\; t.$$

That is, every type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$ that is realised by at least t elements from the $(R{-}r)$-neighbourhood of the set X in $\mathcal{A}$ is still frequent in the substructure of $\mathcal{A}$ induced by deleting the $(R{-}r)$-neighbourhood of X.

In the following, a *disjoint extension* $\mathcal{C}$ of $\mathcal{A}$ (by a structure $\mathcal{D}$) is an extension of $\mathcal{A}$ where there is no edge between any element from A and any element from $C \setminus A$ in the Gaifman graph $\mathcal{G}_{\mathcal{C}}$ of $\mathcal{C}$ (and where $\mathcal{C} - A$ is isomorphic to $\mathcal{D}$).

Consider the following sequences $(\mathcal{C}_i)_{i \geq 0}$ and $(\mathcal{D}_{2i})_{i \geq 1}$ of σ-structures from $\mathfrak{D}$. Let $\mathcal{C}_0 \coloneqq \mathcal{A}$ and $\mathcal{C}_1 \coloneqq \mathcal{A} - X$. For $i \geq 2$, we proceed inductively and distinguish between even and odd numbers i:

(Even i) Here, $\mathcal{D}_i \coloneqq \mathcal{C}_{i-1}[N_{2(i-1)r}^{\mathcal{A}}(X)]$ and $\mathcal{C}_i$ is a disjoint extension of $\mathcal{A}$ by $\mathcal{D}_i$.

(Odd i) For odd i, the structure $\mathcal{D}_i$ is neither defined nor required. On the other hand, $\mathcal{C}_i$ is the union of the disjoint structures $\mathcal{A} - N_{2(i-1)r}^{\mathcal{A}}(X)$ and $\mathcal{D}_{i-1}$.

For a visualisation of the sequence $(\mathcal{C}_i)_{i \geq 0}$, see Figure 6.2. In particular, for all even $i \geq 0$, the structure $\mathcal{C}_i$ is a disjoint extension of $\mathcal{A}$, and for all odd i, the structure $\mathcal{C}_i$ is a proper induced substructure of $\mathcal{A}$. Furthermore, for all $i \in [1,s]$, every element a_j with $j \in [1,n]$ is still present in $\mathcal{C}_i$ and, in particular,

$$\mathcal{N}_r^{\mathcal{C}_i}(\overline{a}) \;\cong\; \mathcal{N}_r^{\mathcal{A}}(\overline{a}). \tag{3}$$

Consider a type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$. Recall that $|X| = t \cdot L$ and that the R-spheres

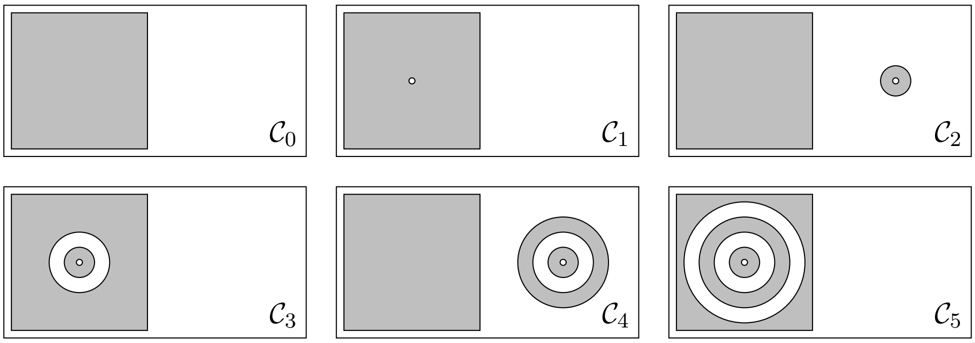

Figure 6.2 The first six elements of the sequence $(\mathcal{C}_i)_{i\geq 0}$. Note that for all even i, $\mathcal{C}_i$ is a disjoint extension of $\mathcal{A}$ while for each odd i, $\mathcal{C}_i$ is a proper induced substructure of $\mathcal{A}$.

around the elements of X in $\mathcal{A}$ are disjoint and isomorphic. This implies that, for each $i \in [1, s)$, there is a number $k \in \mathbb{Z}$ such that

$$|\tau(\mathcal{A} - N^{\mathcal{A}}_{2(i-1)r}(X))| \quad = \quad |\tau(\mathcal{A})| + k \cdot t \cdot L$$

and therefore $|\tau(\mathcal{A} - N^{\mathcal{A}}_{2(i-1)r}(X))|$ and $|\tau(\mathcal{A})|$ are congruent modulo L. Furthermore, since $|X|$ is a multiple of L, it is straightforward to see that also $|\tau(\mathcal{D}_i)|$ is a multiple of L for all even $i \leq s$. This immediately proves the following Claim 1:

Claim 1. *The following holds for all $i < s$ and every type $\tau \in \mathfrak{T}^{d,\sigma}_r(1)$:*

$$|\tau(\mathcal{C}_i)| \;\equiv\; |\tau(\mathcal{C}_{i+1})| \mod L.$$

A proof of the following Claim 2 is deferred to the end of the proof of Theorem 6.2.1.

Claim 2. *The following holds for all $i < s$ and every type $\tau \in \mathfrak{T}^{d,\sigma}_r(1)$:*

(a) If τ is frequent in $\mathcal{C}_i$, it is also frequent in $\mathcal{C}_{i+1}$.

(b) If τ is rare in $\mathcal{C}_i$ and rare in $\mathcal{C}_{i+1}$, then $|\tau(\mathcal{C}_i)| = |\tau(\mathcal{C}_{i+1})|$.

While every type from $\mathfrak{T}^{d,\sigma}_r(1)$ that is frequent in $\mathcal{C}_i$ is also frequent in $\mathcal{C}_{i+1}$, the opposite is not necessarily true: There may be types in $\mathfrak{T}^{d,\sigma}_r(1)$ that are rare in $\mathcal{C}_i$ but that occur frequently in $\mathcal{C}_{i+1}$. However, since there are at most s pairwise non-isomorphic types with radius r and one centre that may be realised in structures from $\mathfrak{D}$, and since $\mathcal{C}_0$ already contains frequent types, Statement (a)

$$\begin{array}{ccccc} & & \mathcal{A} \models \varphi[\overline{a}] & & \\ & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\supseteq$} & \\ \mathcal{B} \models \varphi[\overline{a}] & & \text{iff} & & \mathcal{A}' \models \varphi[\overline{a}] \end{array}$$

Figure 6.3 The illustration shows an overview over the proof of Theorem 6.2.1. Here, the set inclusions suggest that $\mathcal{B}$ and $\mathcal{A}'$ are a disjoint extension and an induced substructure of $\mathcal{A}$, respectively. In particular, there is an $i \geq 0$ such that $\mathcal{A} := \mathcal{C}_i$ and $\mathcal{B} := \mathcal{C}_{i+1}$, or the other way around, so that $(\mathcal{B}, \overline{a})$ and $(\mathcal{A}', \overline{a})$ can not be distinguished by $\varphi(\overline{x})$.

of Claim 2 implies that there has to be an $i < s$ such that all types $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$ that are frequent in $\mathcal{C}_{i+1}$ are already frequent in $\mathcal{C}_i$. Thus, for this particular i we know that any type from $\mathfrak{T}_r^{d,\sigma}(1)$ is either frequent in $\mathcal{C}_{i+1}$ and in $\mathcal{C}_i$ or it is rare in $\mathcal{C}_{i+1}$ and in $\mathcal{C}_i$. Hence, with Statement (b) of Claim 2 it follows that for every type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$, either $|\tau(\mathcal{C}_i)| = |\tau(\mathcal{C}_{i+1})|$ or τ is frequent in $\mathcal{C}_i$ and $\mathcal{C}_{i+1}$.

Together with Isomorphism (3) and Claim 1, we can conclude from Theorem 3.3.1 that

$$\mathcal{C}_i \models \varphi[\overline{a}] \quad \text{iff} \quad \mathcal{C}_{i+1} \models \varphi[\overline{a}].$$

Therefore, by using Claim 2, the proof of Theorem 6.2.1 can be completed as follows: In case that i is even, we let $\mathcal{B} := \mathcal{C}_i$ and $\mathcal{A}' := \mathcal{C}_{i+1}$; and in case that i is odd, we let $\mathcal{B} := \mathcal{C}_{i+1}$ and $\mathcal{A}' := \mathcal{C}_i$. Since $\mathcal{B}$ is a disjoint extension of $\mathcal{A}$ by an induced substructure of $\mathcal{A}$ (and hence belongs to $\mathfrak{D}$, since $\mathfrak{D}$ is closed under disjoint unions and induced substructures), $\mathcal{A} \models \varphi[\overline{a}]$, and $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{D}$, we obtain that $\mathcal{B} \models \varphi[\overline{a}]$. Because $\mathcal{A}' \models \varphi[\overline{a}]$ if and only if $\mathcal{B} \models \varphi[\overline{a}]$, we know that $\mathcal{A}' \models \varphi[\overline{a}]$. Since $\mathcal{A}'$ is a proper induced substructure of $\mathcal{A}$ and $\mathfrak{D}$ is closed under induced substructures, we have $\mathcal{A}' \in \mathfrak{D}$. However, this is a contradiction to the assumption that $(\mathcal{A}, \overline{a})$ is a $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$.

Therefore, every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of size at most $N := (2S \cdot t \cdot L + n - 1) \cdot \nu_d(2R)$. To obtain an upper bound on N in terms of the parameters of $\varphi(\overline{x})$, recall that $S \in S^{d,||\sigma||}(R)$ and $R \in 2r \cdot S^{d,||\sigma||}(r)$. Therefore, since $S^{d,||\sigma||}(r)$ is an abbreviation for the expression $2^{\nu_d(r)^{\mathcal{O}(||\sigma||)}}$, we know that

$$S \in S^{d,||\sigma||}(2 \cdot r \cdot 2^{\nu_d(r)^{\mathcal{O}(||\sigma||)}}) \quad \subseteq \quad S^{d,||\sigma||}(S^{d,||\sigma||}(r)). \tag{4}$$

The latter inclusion is correct since, for each $d \geq 2$, the function ν_d is strictly increasing. Similarly, we have that

$$\nu_d(2R) \quad = \quad \nu_d(2 \cdot 2 \cdot r \cdot 2^{\nu_d(r)^{\mathcal{O}(||\sigma||)}}) \quad \subseteq \quad \nu_d(S^{d,||\sigma||}(r)). \tag{5}$$

Thus, using Estimate (4) and Definition 1, the expression $2S \cdot t \cdot L + n - 1$ can be bounded from above by

$$\begin{aligned} & 2S^{d,||\sigma||}(S^{d,||\sigma||}(r)) \cdot (T + (n{+}q) \cdot \nu_d(r)) \cdot L + n - 1 \\ \subseteq \quad & S^{d,||\sigma||}(S^{d,||\sigma||}(r)) \cdot (T + (n{+}q) \cdot \nu_d(r)) \cdot L \\ \subseteq \quad & S^{d,||\sigma||}(S^{d,||\sigma||}(r)) \cdot (T{+}n{+}q) \cdot L \end{aligned} \tag{6}$$

By putting Estimate (5) and Estimate (6) together, and recalling that $r = 4^q$, we obtain that $N \leq N^{d,||\sigma||}(T, P, n, q, L)$ for

$$\begin{aligned} N^{d,||\sigma||}(T, P, n, q, L) \;\; & \in \;\; S^{d,||\sigma||}(S^{d,||\sigma||}(4^q)) \cdot (T{+}n{+}q) \cdot L \cdot \nu_d(S^{d,||\sigma||}(4^q)) \\ & \subseteq \;\; S^{d,||\sigma||}(S^{d,||\sigma||}(4^q)) \cdot (T{+}n{+}q) \cdot L. \end{aligned}$$

All that remains to be done to finish the proof of Theorem 6.2.1 is to prove Claim 2.

Proof of Claim 2. Observe that for all $i, j \leq s$,

$$\mathcal{C}_i[A \setminus N^{\mathcal{A}}_{R-2r}(X)] \;\cong\; \mathcal{C}_j[A \setminus N^{\mathcal{A}}_{R-2r}(X)]. \tag{7}$$

Let $i < s$. For the proof of Statement (b) of Claim 2, let $\tau \in \mathfrak{T}^{d,\sigma}_r(1)$ be a type that is rare in $\mathcal{C}_i$ and $\mathcal{C}_{i+1}$. Since X is an R-scattered set of size $\geq t$, the rareness of τ implies that $\tau(\mathcal{C}_i)$ and $\tau(\mathcal{C}_{i+1})$ are subsets of $A \setminus N^{\mathcal{A}}_{R-r}(X)$. Hence, Isomorphism (7) implies that $|\tau(\mathcal{C}_i)| = |\tau(\mathcal{C}_{i+1})|$. This proves Statement (b) of Claim 2.

For the proof of Statement (a) of Claim 2, we distinguish between even and odd i.

(Even i) Recall that $\mathcal{C}_0 = \mathcal{A}$ and that for each even $i \geq 2$, the structure $\mathcal{C}_i$ is a disjoint extension of $\mathcal{A}$ by $\mathcal{D}_i$, that is, the union of $\mathcal{A}$ with a structure $\mathcal{D}'_i$ that is isomorphic to $\mathcal{D}_i$ and has an universe disjoint from A. Let τ be a type from $\mathfrak{T}^{d,\sigma}_r(1)$ that is frequent in $\mathcal{C}_i$. In the following, we make a case distinction on the elements of $\mathcal{C}_i$ which realise τ.

(Case 1) Suppose that τ is realised in $\mathcal{C}_i$ by an element in the set $N^{\mathcal{A}}_{R-r}(X)$. Then, τ is realised by at least t elements from $N^{\mathcal{A}}_{R-r}(X)$, since X is R-scattered and $|X| \geq t$. Furthermore,

we obtain from Isomorphism (2) that τ is also realised by at least t elements in the set $N^{\mathcal{A}}_{R-r}(X'\ X)$. Since $X \subseteq X'$, the set X' is R-scattered, and $2i \cdot r < R$, we can conclude that τ is frequent in the structure $\mathcal{A} - N^{\mathcal{A}}_{2i \cdot r}(X)$. Thus, τ is also frequent in $\mathcal{C}_{i+1}$.

(Case 2) Suppose that $i \geq 2$ and τ is realised by an element of $\mathcal{D}'_i$. Since $\mathcal{D}'_i \cong \mathcal{D}_i$, the type τ is also realised by an element from $D_i \subseteq N^{\mathcal{A}}_{R-r}(X)$ in $\mathcal{C}_{i+1}$. Thus, τ is also frequent in $\mathcal{C}_{i+1}$.

(Case 3) Otherwise, we know that τ is already realised by at least t elements from A that do not belong to $N^{\mathcal{A}}_{R-r}(X)$. Then, it follows from Isomorphism (7) that τ is also frequent in $\mathcal{C}_{i+1}$.

(Odd i) Recall that $\mathcal{C}_1 = \mathcal{A} - X$ and that, for each odd $i \geq 3$, the structure $\mathcal{C}_i$ is the union of $\mathcal{A} - N^{\mathcal{A}}_{2(i-1)\cdot r}(X)$ and $\mathcal{D}_{i-1}$. Let τ be a type from $\mathfrak{T}^{d,\sigma}_r(1)$ that is frequent in $\mathcal{C}_i$. Again, we make a case distinction on the elements of $\mathcal{C}_i$ which realise τ.

(Case 1) Suppose that τ is in $\mathcal{C}_i$ realised by an element from the set $N^{\mathcal{A}}_{2(i-1)\cdot r+r}(X)$. Since X is R-scattered and $|X| \geq t$, at least t elements from $N^{\mathcal{A}}_{2(i-1)\cdot r+r}(X)$ realise τ in $\mathcal{C}_i$. As $\mathcal{D}_{i+1}$ is the structure $\mathcal{C}_i[N^{\mathcal{A}}_{2(i-1)\cdot r+2r}(X)]$, we can conclude that τ is frequent in $\mathcal{D}_{i+1}$. Then, τ is also frequent in $\mathcal{C}_{i+1}$, since $\mathcal{C}_{i+1}$ is the disjoint extension of $\mathcal{A}$ by $\mathcal{D}_{i+1}$.

(Case 2) Otherwise, we know that in $\mathcal{C}_i$, the type τ is realised by at least t elements from $A \setminus N^{\mathcal{A}}_{2(i-1)\cdot r+r}(X)$. However, since the r-sphere of each element $a \in A \setminus N^{\mathcal{A}}_{2(i-1)\cdot r+r}(X)$ in the structure $\mathcal{A} - N^{\mathcal{A}}_{2(i-1)\cdot r}(X)$ is isomorphic to its r-sphere in $\mathcal{A}$, and $\mathcal{C}_{i+1}$ is a disjoint extension of $\mathcal{A}$ by $\mathcal{D}_{i+1}$, the type τ is also frequent in $\mathcal{C}_{i+1}$.

This concludes the proof of Claim 2 and Theorem 6.2.1. $\square$

For proving Theorem 6.1.7, it remains to do the following: for a given formula $\varphi(\overline{x})$ from FO+unM$[\sigma]$ that is preserved under extensions on $\mathfrak{D}$ and for an upper bound on the size of its $\mathfrak{D}$-minimal models, obtained from Theorem 6.2.1, construct an existential formula from $\mathsf{FO}[\sigma]$ that is $\mathfrak{D}$-equivalent to $\varphi(\overline{x})$. This is done by using the following lemma, which is a generalisation of Lemma 8.4 in [DGKS07] to formulae (possibly with free variables) with modulo-counting quantifiers.

Lemma 6.2.2. *There is an algorithm which, on input of*

- *a number $N \geq 1$ and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$ over a relational signature σ,*

constructs an existential formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ such that the following holds for every class $\mathfrak{C}$ of σ-structures that is closed under induced substructures:

If $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{C}$ and every $\mathfrak{C}$-minimal model of $\varphi(\overline{x})$ has a universe of size $\leq N$, then $\psi(\overline{x})$ is $\mathfrak{C}$-equivalent to $\varphi(\overline{x})$.

Furthermore, the algorithm constructs $\psi(\overline{x})$ in time

$$||\varphi|| \cdot (2\max\{1, T, P\})^{(n+q)\cdot\mathcal{O}(\log N)},$$

where $T, P, q \geq 0$ are the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$. The constant suppressed by the $\mathcal{O}$-notation does not depend on the signature σ.

The key ingredient for the proof of Lemma 6.2.2 is contained in the following lemma. Here, an *enumeration of a set A* is a tuple $(e_1, \ldots, e_M) \in A^M$ of length $M = |A|$ that contains each element of A exactly once, that is, $A = \{e_1, \ldots, e_M\}$.

Lemma 6.2.3. *Let σ be a relational signature, let $m \geq 0$, and let $\varphi(x_1, \ldots, x_m)$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$ where all variables occurring in φ are among $x_1, \ldots, x_m$.*

For each $M \geq 1$ and every function $s\colon [1, m] \to [1, M]$, there is a quantifier-free formula $(\varphi)_{M,s}(y_1, \ldots, y_M)$ from $\mathsf{FO}[\sigma]$ such that for each σ-structure $\mathcal{A}$ with exactly M elements and every enumeration $(e_1, \ldots, e_M)$ of A,

$$\begin{array}{rcl} \mathcal{A} & \models & \varphi[e_{s(1)}, \ldots, e_{s(m)}] \\ \textit{iff} \quad \mathcal{A} & \models & (\varphi)_{M,s}[e_1, \ldots, e_M]. \end{array}$$

Furthermore, there is an algorithm which, on input of $\varphi(\overline{x})$, M, and s, constructs $(\varphi)_{M,s}$ in time

$$\mathcal{O}(||\varphi||) \cdot (2\max\{T, P\})^{q\cdot\mathcal{O}(\log M)},$$

where $T, P, q \geq 0$ are the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$. The constants suppressed by the $\mathcal{O}$-notation do not depend on the signature σ.

Before presenting the proof of Lemma 6.2.3, we first show how to use Lemma 6.2.3 for proving Lemma 6.2.2.

Proof of Lemma 6.2.2 using Lemma 6.2.3. Let σ be a relational signature, let $N \geq 1$, and let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$, where $\overline{x} = (x_1, \dots, x_n)$ are the $n \geq 0$ free variables of ψ. Furthermore, choose $m \geq n$ such that *all* variables that occur in $\varphi(\overline{x})$ are among the variables $x_1, \dots, x_n, x_{n+1}, \dots, x_m$.

For each $M \in [1, N]$, let S be the set of all functions $s \colon [1, m] \to [1, M]$ with $s(i) = 1$ for all $i \in [n{+}1, m]$, and choose

$$\psi_M(x_1, \dots, x_n, y_1, \dots, y_M) \;\coloneqq\; \bigwedge_{1 \leq i < j \leq M} \neg y_i{=}y_j \quad \wedge$$
$$\bigvee_{s \in S} \Bigg(\bigwedge_{i=1}^{n} x_i{=}y_{s(i)} \quad \wedge \quad (\varphi)_{M,s}(y_1, \dots, y_M) \Bigg).$$

Using the formulae $\psi_M(x_1, \dots, x_n, y_1, \dots, y_M)$ for $M \in [1, N]$, we let

$$\psi(\overline{x}) \;\coloneqq\; \bigvee_{M=1}^{N} \exists y_1 \cdots \exists y_M \, \psi_M(\overline{x}, y_1, \dots, y_M).$$

The following claim shows that the formula $\psi(\overline{x})$ indeed satisfies the conditions required by Lemma 6.2.2.

Claim 1. *Let $\mathfrak{C}$ be a class of σ-structures that is closed under induced substructures, and suppose that $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{C}$. Furthermore, suppose that every $\mathfrak{C}$-minimal model of $\varphi(\overline{x})$ has a universe of size $\leq N$. Then, for each $\mathcal{A} \in \mathfrak{C}$ and every tuple $\overline{a} \in A^n$,*

$$\mathcal{A} \models \varphi[\overline{a}] \quad \textit{iff} \quad \mathcal{A} \models \psi[\overline{a}].$$

Proof of Claim 1. Let $\mathcal{A} \in \mathfrak{C}$ and let $\overline{a} = (a_1, \dots, a_n) \in A^n$. We prove the two directions of the equivalence.

For the 'only if" direction, suppose that $\mathcal{A} \models \varphi[\overline{a}]$. Since $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{C}$ and the universe of every $\mathfrak{C}$-minimal model of $\varphi(\overline{x})$ has at most N elements, there is an induced substructure $\mathcal{A}' \in \mathfrak{C}$ of $\mathcal{A}$ with a universe A' of exactly $M \in [1, N]$ pairwise distinct elements $e_1, \dots, e_M$, such that $\{a_1, \dots, a_n\} \subseteq A'$ and $\mathcal{A}' \models \varphi[\overline{a}]$.

As the variables $x_{n+1}, \dots, x_m$ are not free in $\varphi(\overline{x})$, this implies that also $\mathcal{A}' \models \varphi[e_{s(1)}, \dots, e_{s(m)}]$ for the function $s \in S$ where $e_{s(i)} = a_i$ for all $i \in [1, n]$. By Lemma 6.2.3, we know that $\mathcal{A}' \models (\varphi)_{M,s}[e_1, \dots, e_M]$ and thus, since $e_1, \dots, e_M$ are pairwise distinct, that $\mathcal{A}' \models \psi_M[\overline{a}, e_1, \dots, e_M]$.

Therefore, by assigning each of the variables y_i for $i \in [1, M]$ with the corresponding element e_i, we can conclude that $(\mathcal{A}', \overline{a}) \models \exists y_1 \cdots \exists y_M \, \psi_M(\overline{x}, y_1, \dots, y_M)$

and thus, also $\mathcal{A}' \models \psi[\overline{a}]$. Observe that $\psi(\overline{x})$ is an existential formula and therefore, in particular, preserved under extensions on $\mathfrak{C}$. It follows that $\mathcal{A} \models \psi[\overline{a}]$.

For the "if" direction, suppose that $\mathcal{A} \models \psi[\overline{a}]$. Then, there is an $M \in [1, N]$ and a substructure $\mathcal{A}' \in \mathfrak{C}$ of $\mathcal{A}$, induced by pairwise distinct elements $e_1, \ldots, e_M$ from A, such that $\{a_1, \ldots, a_n\} \subseteq A'$ and such that $\mathcal{A}' \models (\varphi)_{M,s}[e_1, \ldots, e_M]$ for the function $s \in S$ where $e_{s(i)} = a_i$ for all $i \in [1, n]$.

It follows from Lemma 6.2.3 that $\mathcal{A}' \models \varphi[e_{s(1)}, \ldots, e_{s(m)}]$ and thus, by choice of the function s and since $x_{n+1}, \ldots, x_m$ are not free in $\varphi(\overline{x})$, also $\mathcal{A}' \models \varphi[\overline{a}]$. As $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{C}$, we can conclude that $\mathcal{A} \models \varphi[\overline{a}]$.

This completes the proof of Claim 1.

Time complexity. Let $T, P, q \geq 0$ be the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$, respectively.

We first estimate the time required for the construction of the formulae $\psi_M(\overline{x}, y_1, \ldots, y_M)$ for $M \in [1, N]$. Observe that the set S has cardinality M^n. Since, by Lemma 6.2.3, each formula $(\varphi)_{M,s}(y_1, \ldots, y_M)$ with $s \in S$ has size in

$$\mathcal{O}(||\varphi||) \cdot (2 \max\{T, P\})^{q \cdot \mathcal{O}(\log M)},$$

the formula $\psi_M(\overline{x}, y_1, \ldots, y_M)$ can be computed in time

$$\begin{aligned} & \mathcal{O}(M^2) + M^n \cdot \left(\mathcal{O}(n) + \mathcal{O}(||\varphi||) \cdot (2 \max\{T, P\})^{q \cdot \mathcal{O}(\log M)}\right) \\ \subseteq \quad & ||\varphi|| \cdot (2 \max\{1, T, P\})^{(n+q) \cdot \mathcal{O}(\log M)}. \end{aligned}$$

For the latter inclusion, recall that $q + n \geq 1$.

Since $\psi(\overline{x})$ is the disjunction of all formulae $\exists y_1 \cdots \exists y_m \, \psi_M(\overline{x}, y_1, \ldots, y_M)$ for $M \in [1, N]$, it can thus be constructed within time

$$\begin{aligned} & N \cdot \left(\mathcal{O}(N) + ||\varphi|| \cdot (2 \max\{1, T, P\})^{(n+q) \cdot \mathcal{O}(\log N)}\right) \\ \subseteq \quad & ||\varphi|| \cdot (2 \max\{1, T, P\})^{(n+q) \cdot \mathcal{O}(\log N)}. \end{aligned}$$

This completes the proof of Lemma 6.2.2. $\square$

Proof of Lemma 6.2.3. Let σ be a relational signature, let $m \geq 0$, and let furthermore $\varphi(x_1, \ldots, x_m)$ be a formula from $\mathsf{FO{+}unM}[\sigma]$ whose variables, including the quantified ones, are all among $x_1, \ldots, x_m$.

Moreover, let $M \geq 1$ and let $s\colon [1, m] \to [1, M]$. The construction of the quantifier-free formula $(\varphi)_{M,s}(y_1, \ldots, y_M)$ from $\varphi(x_1, \ldots, x_m)$ proceeds by induction on the shape of φ.

If $\varphi(x_1, \dots, x_m)$ *is an atomic formula*, then $(\varphi)_{M,s}$ is the formula obtained by replacing all occurrences of each variable x_i for $i \in [1, m]$ in $\varphi(x_1, \dots, x_m)$ by the variable $y_{s(i)}$. It is straightforward to verify that $(\varphi)_{M,s}(y_1, \dots, y_M)$ satisfies the condition of Lemma 6.2.3:

In particular, if $\varphi(x_1, \dots, x_m)$ is of the shape $R(x_{i_1}, \dots, x_{i_r})$ for a relation symbol R from σ with arity $r \geq 1$ and for suitable indices $i_1, \dots, i_r \in [1, m]$, we let

$$(\varphi)_{M,s}(y_1, \dots, y_M) \;\; := \quad R(y_{s(i_1)}, \dots, y_{s(i_r)}).$$

Then, for each σ-structure $\mathcal{A}$ with at most M elements and for every enumeration $(e_1, \dots, e_M)$ of A, the following equivalences show that the condition of Lemma 6.2.3 is satisfied:

$$\mathcal{A} \models \varphi[e_{s(1)}, \dots, e_{s(m)}] \;\text{ iff }\; (e_{s(i_1)}, \dots, e_{s(i_r)}) \in R^{\mathcal{A}} \;\text{ iff }\; \mathcal{A} \models (\varphi)_{M,s}[e_1, \dots, e_M].$$

For $\varphi(x_1, \dots, x_m)$ of the shape $x_i{=}x_j$ with $i, j \in [1, m]$, analogous equivalences hold.

For a Boolean combination $\varphi(x_1, \dots, x_m)$, the translation distributes. For $\varphi = \neg\psi$ we let $(\varphi)_{M,s} := \neg(\psi)_{M,s}$, and for $\varphi = (\psi \vee \psi')$ we let $(\varphi)_{M,s} := (\psi)_{M,s} \vee (\psi')_{M,s}$. In both cases, the condition of Lemma 6.2.3 is clearly satisfied.

Suppose that $\varphi(x_1, \dots, x_m)$ *is of the shape* $(\mathsf{Q}{+}k)x_i\, \psi(x_1, \dots, x_m)$ for a quantifier $\mathsf{Q} \in D_{\text{all}} \cup \{\exists\}$ and $k \geq 0$.

For $i \in [1, m]$ and $j \in [1, M]$, we denote in the following by $s[i \to j]$ the function $s'\colon [1, m] \to [1, M]$ with $s'[i] = j$ and $s'[i'] = s[i']$ for all $i' \in [1, m]$, $i' \neq i$. For every $j \in [1, M]$, we consider the formula $(\psi)_{M,s[i \to j]}(y_1, \dots, y_M)$, for which the following holds: If $\mathcal{A}$ is a σ-structure with precisely M elements and $(e_1, \dots, e_M)$ is an enumeration of A, then

$$\begin{array}{rcl} \mathcal{A} & \models & \psi[e_{s(1)}, \dots, e_{s(i-1)}, e_j, e_{s(i+1)}, \dots, e_{s(m)}] \\ \text{iff} \;\; \mathcal{A} & \models & (\psi)_{M,s[i \to j]}[e_1, \dots, e_M]. \end{array}$$

Our aim is thus to construct a formula $(\varphi)_{M,s}(x_1, \dots, x_M)$, such that

$$\begin{array}{rl} & \mathcal{A} \;\models\; (\varphi)_{M,s}[e_1, \dots, e_M] \\ \text{iff} & |\{j \in [1, M] \,:\, \mathcal{A} \models (\psi)_{M,s[i \to j]}[e_1, \dots, e_M]\}| \;\in\; (\mathsf{Q}{+}k) \end{array} \tag{1}$$

for every σ-structure $\mathcal{A}$ with precisely M elements and each enumeration $(e_1, \dots, e_M)$ of A.

We use the observations of Section 2.9 for an inductive construction of $(\varphi)_{M,s}(y_1, \dots, y_M)$, whose size only grows polynomially with M. To this aim, we distinguish between the cases of Q being a modulo-counting or the existential quantifier. In both cases, we let $\bot := \neg y_1{=}y_1$ an unsatisfiable formula.[1]

(Case 1) *If* $(\mathsf{Q}{+}k) = \exists^{\equiv k \bmod p}$ *for* $p \geq 2$ *and* $k \in [0, p)$, we let

$$\delta_j^{\equiv \ell \bmod p}(y_1, \ldots, y_M) \;:=\; \begin{cases} \neg(\psi)_{M,s[i \to j]} & \text{if } \ell = 0, \\ (\psi)_{M,s[i \to j]} & \text{if } \ell = 1, \text{ and} \\ \bot & \text{otherwise.} \end{cases}$$

for each $\ell \in [0, p)$ and $j \in [1, M]$. Consider the formula

$$\bigvee_{f \in F} \bigwedge_{j \in M} \delta_j^{\equiv f(j) \bmod p}(y_1, \ldots, y_M)$$

where F is the set of all functions $f\colon M \to [0, p)$ such that the sum of the values $f(j)$ for all $j \in M$ is congruent to k modulo p. Although this formula satisfies Equivalence (1), it grows exponentially with M.

However, by Lemma 2.9.2, the formula is equivalent to the Boolean combination

$$(\varphi)_{M,s}(y_1, \ldots, y_M) \;:=\; \langle \delta_j^{\equiv \ell \bmod p} \rangle_M^{\equiv k \bmod p}(y_1, \ldots, y_M)$$

of formulae $\delta_j^{\equiv \ell \bmod p}(y_1, \ldots, y_M)$ with $\ell \in [0, p)$ and $j \in M$.

(Case 2) *If* $(\mathsf{Q}{+}k) = \exists^{>k}$, we proceed similarly and let

$$\delta_j^{>\ell}(y_1, \ldots, y_M) \;:=\; \begin{cases} (\psi)_{M,s[i \to j]} & \text{if } \ell = 0, \text{ and} \\ \bot & \text{otherwise.} \end{cases}$$

for all $\ell \in [0, k]$ and $j \in M$. The formula

$$\bigvee_{g \in G} \bigwedge_{\substack{j \in M, \\ g(j) \geq 0}} \delta_j^{>g(j)}(y_1, \ldots, y_M)$$

where G is the set of all functions $g\colon M \to [-1, k]$, such that the sum of the values $g(j) + 1$ for all $j \in M$ adds up to $k + 1$, satisfies Equivalence (1). Since also this formula grows exponentially with M, we replace it again by the equivalent formula

$$(\varphi)_{M,s}(y_1, \ldots, y_M) \;:=\; \langle \delta_j^{>\ell} \rangle_M^{>k}(y_1, \ldots, y_M)$$

defined in Lemma 2.9.4, which is, in particular, a Boolean combination of formulae $\delta_j^{>\ell}(y_1, \ldots, y_M)$ with $\ell \in [0, k]$ and $j \in M$.

[1] The formula $\bot$ introduced here should not be mistaken for the symbol $\bot$ representing an unsatisfiable existential-positive sentence.

We complete the proof of Lemma 6.2.3 by providing an analysis of the time required for constructing the formula $(\varphi)_{M,s}(y_1, \dots, y_M)$.

Time complexity. In the following, we let $T, P, q \geq 0$ the threshold, the maximum period, and the quantifier rank of φ.

The only size increasing steps in the inductive translation are the ones for quantifiers, that is, subformulae of the shape $(\mathsf{Q}{+}k)x_i\,\psi$. Summing up the time needed for the case of $(\mathsf{Q}{+}k) = \exists^{\equiv k \bmod p}$ for $p \in [2, P]$ and $k \in [0, p)$, and for the case of $(\mathsf{Q}{+}k) = \exists^{>k}$ with $k \in [0, T]$, this increases the size of the formula by a factor of $(2\max\{T, P\})^{\mathcal{O}(\log M)}$, according to Lemma 2.9.2 and Lemma 2.9.4, respectively. Thus,

$$||(\varphi)_{M,s}|| \;\in\; \mathcal{O}(||\varphi||) \cdot (2\max\{T, P\})^{q \cdot \mathcal{O}(\log M)}.$$

It is easy to see that the time required for the construction of $(\varphi)_{M,s}(y_1, \dots, y_M)$ can be bounded by the same expression. This completes the proof of Lemma 6.2.3. □

Theorem 6.1.7 is now obtained by a straightforward combination of Theorem 6.2.1 and Lemma 6.2.2.

Proof of Theorem 6.1.7. Let $d \geq 2$ be a degree bound, let σ be a relational signature, and let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$ with $n := |\overline{x}|$ free variables, threshold $T \geq 0$, maximum period $P \geq 0$, and quantifier rank $q \geq 0$. Furthermore, let $L \geq 1$ be the least common multiple of the periods of all modulo-counting quantifiers occurring in $\varphi(\overline{x})$.

Let $\mathfrak{D}$ be a class of d-bounded σ-structures that is closed under disjoint unions and induced substructures and suppose that $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{D}$.

The algorithm proceeds in the following two steps:

(Step 1) Compute the upper bound

$$\begin{aligned} N \;&:=\; N^{d,||\sigma||}(T, n, q, L) \\ &\in\; S^{d,||\sigma||}(S^{d,||\sigma||}(4^q)) \cdot (T{+}n{+}q) \cdot L \qquad (1) \end{aligned}$$

on the size of $\mathfrak{D}$-minimal models of $\varphi(\overline{x})$, obtained from Theorem 6.2.1. In particular, we can assume that $N \geq 2$.

(Step 2) The algorithm of Lemma 6.2.2 constructs an existential formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ that is $\mathfrak{D}$-equivalent to $\varphi(\overline{x})$. This takes time in

$$\begin{aligned} & \mathcal{O}(||\varphi||) \cdot (2\max\{1,T,P\})^{(n+q)\cdot\mathcal{O}(\log N)} \\ \subseteq \quad & ||\varphi|| \cdot N^{(n+q)\cdot\mathcal{O}(\log\max\{1,T,P\})} \end{aligned}$$

Thus, by replacing N in the latter estimate with Estimate (1) and recalling the definition of $S^{\cdot,\cdot}(\cdot)$, we obtain that $\psi(\overline{x})$ can altogether be computed in time

$$||\varphi|| \cdot \Big(2^{\nu_d(2^{\nu_d(4^q)^{\mathcal{O}(||\sigma||)}})} \cdot (T{+}n{+}q) \cdot L\Big)^{(n+q)\cdot\mathcal{O}(\log\max\{1,T,P\})}.$$

This completes the proof of Theorem 6.1.7. □

6.3 Preservation under Homomorphisms

This section is devoted to the proof of Theorem 6.1.10, whose combinatorial essence is contained in the following Theorem 6.3.1. Further down below, Lemma 6.3.2 uses this upper bound on the size of minimal models of formulae that are preserved under homomorphisms, to construct existential-positive formulae. The section concludes with the actual proof of Theorem 6.1.10, which combines the aforementioned steps.

Theorem 6.3.1. *There is a function $N\colon \mathbb{N}^4 \to \mathbb{N}$ with*

$$N^{d,||\sigma||}(n,q) \quad \in \quad (n{+}1) \cdot S^{d,||\sigma||}(2 \cdot 4^q)$$

such that the following holds for every relational signature σ, every degree bound $d \geq 2$, every class $\mathfrak{D}$ of d-bounded σ-structures that is closed under disjoint unions and induced substructures, and every formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{unM}[\sigma]$:

If $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, then every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of size at most $N^{d,||\sigma||}(n,q)$, where $n, q \geq 0$ are the number of free variables and the quantifier rank of $\varphi(\overline{x})$, respectively.

Note that, in contrast to Theorem 6.2.1, the upper bound on the size of the universe of $\mathfrak{D}$-minimal models for a formula φ that is preserved under homomorphisms on $\mathfrak{D}$ neither depends on the threshold nor on the periods of the quantifiers in φ.

Proof of Theorem 6.3.1. The proof is similar to the proof of Lemma 7.1 in [AG94]. However, it does not rely on Gaifman's theorem but uses the generalisation of Nurmonen's theorem to $\mathsf{FO}{+}\mathsf{unM}$, stated in Theorem 3.3.1.

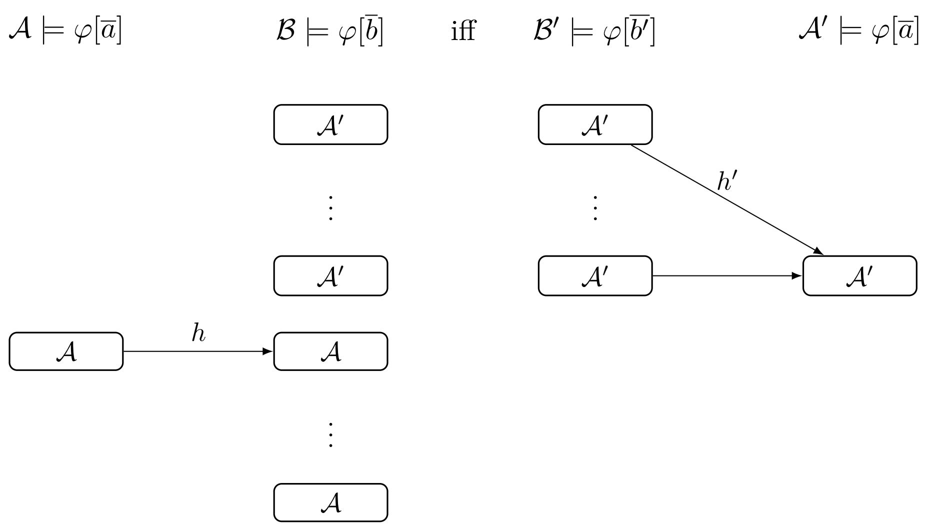

Figure 6.4 The illustration shows an overview over the proof of Theorem 6.3.1. Here, h and h' are homomorphisms from $\mathcal{A}$ to $\mathcal{B}$ and from $\mathcal{B}'$ to the induced substructure $\mathcal{A}'$ of $\mathcal{A}$, respectively. The structures $\mathcal{B}$ and $\mathcal{B}'$ are constructed such that $(\mathcal{B}, \overline{b})$ and $(\mathcal{B}', \overline{b}')$ can not be distinguished by $\varphi(\overline{x})$.

Let σ be a relational signature, let $d \geq 2$, and let $\mathfrak{D}$ be a class of d-bounded σ-structures that is closed under disjoint unions and induced substructures. Furthermore, let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$ with $n := |\overline{x}|$ free variables, and quantifier rank $q \geq 0$. Suppose that $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$.

Let $r := 4^q$ and let $s \in S^{d,||\sigma||}(2r)$ be the number of σ-types with radius $2r$ and one centre that may be realised in structures from $\mathfrak{D}$.

Towards a contradiction, assume that $\varphi(\overline{x})$ has a $\mathfrak{D}$-minimal model $(\mathcal{A}, \overline{a})$ with a universe of size

$$|A| \;>\; (s{+}n) \cdot \nu_d(4r).$$

By Lemma 6.1.14, $\mathcal{A}$ contains a $2r$-scattered set of size $s{+}n{+}1$. Thus, since there are at most s non-isomorphic types with radius $2r$ and one centre realised in $\mathcal{A}$, there must be two elements c_1, c_2 in A whose $2r$-neighbourhoods are disjoint and isomorphic, and do not contain any of the elements in the tuple $\overline{a}$.

Let $\mathcal{A}' := \mathcal{A} - \{c_1\}$. Since $\mathfrak{D}$ is closed under taking induced substructures, also $\mathcal{A}' \in \mathfrak{D}$. Clearly, the r-spheres of elements in $A \setminus N_r^{\mathcal{A}}(c_1)$ are the same in $\mathcal{A}$ and $\mathcal{A}'$. On the other hand, the r-sphere of an element in $N_r^{\mathcal{A}}(c_1)$ might change when moving from $\mathcal{A}$ to $\mathcal{A}'$. However, by our choice of c_1 and c_2 we know that every r-sphere that is realised in $\mathcal{A}$ is also realised in $\mathcal{A}'$: For elements outside the r-neighbourhood of c_1 this is obvious; and for elements $c_1' \in N_r^{\mathcal{A}}(c_1)$, the r-sphere of c_1' in $\mathcal{A}$ is realised in $\mathcal{A}'$ by the corresponding element $c_2' \in N_r^{\mathcal{A}'}(c_2)$.

In the following, we will use Theorem 3.3.1 to show that also $\mathcal{A}' \models \varphi[\overline{a}]$. The argumentation is sketched in Figure 6.4. Let $L \geq 1$ denote the least common multiple of the periods of all modulo-counting quantifiers that occur in $\varphi(\overline{x})$, and let $t := T + (n+q) \cdot \nu_d(r)$, where $T \geq 0$ is the threshold of φ, denote the number chosen in Condition (3) of Theorem 3.3.1 for the degree bound d.

Let $\mathcal{B}$ be a disjoint union of $t \cdot L$ copies of $\mathcal{A}$ and $t \cdot L$ copies of $\mathcal{A}'$. Since $\mathfrak{D}$ is closed under taking disjoint unions, we know that $\mathcal{B} \in \mathfrak{D}$. Obviously, there is an injective homomorphism h that maps $\mathcal{A}$ to one of the copies of $\mathcal{A}$ in $\mathcal{B}$. Since $\mathcal{A} \models \varphi[\overline{a}]$ and $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, we thus obtain that $\mathcal{B} \models \varphi[\overline{b}]$ for $\overline{b} = h(\overline{a})$. Furthermore, $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \mathcal{N}_r^{\mathcal{B}}(\overline{b})$.

Now let $\mathcal{B}'$ be a disjoint union of $t \cdot L$ copies of $\mathcal{A}'$. Since $\mathfrak{D}$ is closed under taking disjoint unions, also $\mathcal{B}' \in \mathfrak{D}$. By construction of $\mathcal{B}$ and $\mathcal{B}'$, every one-centred σ-type τ with radius r is realised in $\mathcal{B}$ if it is realised in $\mathcal{B}'$, and vice versa. Furthermore, the number of realisations of τ in $\mathcal{B}$ or $\mathcal{B}'$ is a multiple of $t \cdot L$. Consider an arbitrary disjoint copy of $\mathcal{A}'$ in $\mathcal{B}'$, and let $\overline{b}'$ be the tuple of elements of this copy corresponding to the tuple $\overline{a}$ in $\mathcal{A}$. In particular, $\mathcal{N}_r^{\mathcal{B}}(\overline{b}) \cong \mathcal{N}_r^{\mathcal{B}'}(\overline{b}')$. Thus, the interpretations $(\mathcal{B}, \overline{b})$ and $(\mathcal{B}', \overline{b}')$ for $\varphi(\overline{x})$ satisfy the assumptions of Theorem 3.3.1, and, since $\mathcal{B} \models \varphi[\overline{b}]$, in particular also $\mathcal{B}' \models \varphi[\overline{b}']$.

By mapping each element of each disjoint copy of $\mathcal{A}'$ in $\mathcal{B}'$ to the corresponding element in $\mathcal{A}'$, we obtain an injective homomorphism h' from $\mathcal{B}'$ to $\mathcal{A}'$ such that, in particular, $h'(\overline{b}') = \overline{a}$. Since $\mathcal{B}' \models \varphi[\overline{b}']$ and $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, we obtain that also $\mathcal{A}' \models \varphi[\overline{a}]$.

This, however, contradicts our assumption that $(\mathcal{A}, \overline{a})$ is a $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$. Therefore, every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of size $N \leq (s+n) \cdot \nu_d(4r)$. Recalling that $r = 4^q$, we obtain that $N \leq N^{d,||\sigma||}(n,q)$ for

$$\begin{aligned} N^{d,||\sigma||}(n,q) &\in (S^{d,||\sigma||}(2 \cdot 4^q) + n) \cdot \nu_d(4 \cdot 4^q) \\ &\subseteq (n+1) \cdot S^{d,||\sigma||}(2 \cdot 4^q). \end{aligned}$$

This concludes the proof of Theorem 6.3.1. $\square$

In the following Lemma 6.3.2, we construct existential-positive $\mathsf{FO}[\sigma]$-formulae for formulae from an arbitrary ultimately periodic logic $\mathsf{L}[\sigma]$ that are preserved under homomorphisms on an arbitrary decidable class of σ-structures. In particular, this includes the logic $\mathsf{FO}+\mathrm{unM}[\sigma]$.

Note that the lemma is stated in a more general way than actually needed for the proof of Theorem 6.1.10, where we only have to consider decidable classes of σ-structures of bounded degree that are closed under disjoint unions and induced substructures and only input formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$. However, the generalisation to formulae from arbitrary ultimately periodic logics $\mathsf{L}[\sigma]$ will be used later in Section 7.5 and Section 8.6.

The proof of Lemma 6.3.2 is an algorithmic version of the proof of Theorem 3.1 in [ADK06].

Lemma 6.3.2. *Let L be an ultimately periodic logic and let $\mathfrak{C}'$ be a class of structures that is decidable in time $t(n)$ for some function $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$.*

There is an algorithm which, on input of

- *a relational signature σ,*
- *a number $N \geq 2$, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{L}[\sigma]$ with $n := |\overline{x}|$ free variables,*

constructs an existential-positive formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$, such that the following holds for the class $\mathfrak{D}$ of all σ-structures from $\mathfrak{C}'$:

If $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$ and every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of size at most N, then $\psi(\overline{x})$ is $\mathfrak{D}$-equivalent to $\varphi(\overline{x})$.

Furthermore, the algorithm constructs $\psi(\overline{x})$ in time

$$2^{||\varphi||\cdot N^{\mathcal{O}(||\sigma||)}} \cdot t(N^{\mathcal{O}(||\sigma||)})$$

and $\psi(\overline{x})$ has size in

$$2^{(n+1)\cdot N^{\mathcal{O}(||\sigma||)}}.$$

The following theorem, well-known as the Chandra-Merlin theorem [CM77] (cf., [AHV95]) is crucial for the construction of existential-positive formulae in Lemma 6.3.2. For its statement, we require some more notation:

Let $\mathcal{A}$ be a σ-structure. Without loss of generality, we assume that the universe of A is a subset of the natural numbers of cardinality $M \geq 1$. That is, the universe of $\mathcal{A}$ consists of M elements $e_1, \ldots, e_M \in \mathbb{N}$ with $e_1 < \cdots < e_M$. Furthermore, let $\overline{a} = (e_{j_1}, \ldots, e_{j_n}) \in A^n$ for indices $j_1, \ldots, j_n \in [1, M]$ be a tuple of $n \geq 0$ elements from A. The *canonical conjunctive query associated with* $(\mathcal{A}, \overline{a})$ is the $\mathsf{FO}[\sigma]$-formula

$$\gamma_{(\mathcal{A},\overline{a})}(x_1, \ldots, x_n) \;:=\; \exists y_1 \cdots \exists y_M \left(\bigwedge_{i=1}^{n} x_i{=}y_{j_i} \;\wedge\; \delta_{\mathcal{A}}(y_1, \ldots, y_M) \right),$$

where $\delta_{\mathcal{A}}(y_1, \ldots, y_M)$ is the conjunction of all atomic formulae of the form $R(y_{i_1}, \ldots, y_{i_r})$ with a relation symbol R from σ of arity $r \geq 1$ and indices $i_1, \ldots, i_r \in [1, M]$, for which $(e_{i_1}, \ldots, e_{i_r}) \in R^{\mathcal{A}}$.

Theorem 6.3.3 ([CM77, AHV95]). *Let σ be a relational signature, let $\mathcal{A}$ and $\mathcal{B}$ be σ-structures, and let $\overline{a} \in A^n$ and $\overline{b} \in B^n$ be tuples of length $n \geq 0$. The following equivalence holds:*

$\mathcal{B} \models \gamma_{(\mathcal{A},\overline{a})}[\overline{b}]$

iff *there is a homomorphism h from $\mathcal{A}$ to $\mathcal{B}$ where $\overline{b} = h(\overline{a})$.*

Before giving a proof of Theorem 6.3.3, we first show how Theorem 6.3.3 is used for the proof of Lemma 6.3.2.

Proof of Lemma 6.3.2 using Theorem 6.3.3. Let L be an ultimately periodic logic and let $\mathfrak{C}'$ be a class of structures that is decidable in time $t(n)$ for some function $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$. Let σ be a relational signature and let $\mathfrak{D}$ be the class of *all* σ-structures from $\mathfrak{C}'$. Furthermore, let $N \geq 2$ and let $\varphi(\overline{x})$ be a formula from $\mathsf{L}[\sigma]$ with $n := |\overline{x}|$ free variables.

The algorithm proceeds along the following steps:

(Step 1) Compute the set $\mathfrak{K}$ that consists of all tuples $(\mathcal{A}, \overline{a})$ with $\mathcal{A} \in \mathfrak{D}$ and $\overline{a} \in A^n$, such that $A = [1, M]$ for an $M \leq N$ and $\mathcal{A} \models \varphi[\overline{a}]$.

(Step 2) If $\mathfrak{K} = \emptyset$, output $\psi := \bot$. Otherwise, that is, if $\mathfrak{K} \neq \emptyset$, output the formula

$$\psi(\overline{x}) \;:=\; \bigvee_{(\mathcal{A},\overline{a})\in\mathfrak{K}} \gamma_{(\mathcal{A},\overline{a})}(\overline{x})$$

Obviously, $\psi(\overline{x})$ is an existential-positive formula from $\mathsf{FO}[\sigma]$.

Before giving details on the algorithm's Step (1) and its running time, let us first show that $\psi(\overline{x})$ is $\mathfrak{D}$-equivalent to $\varphi(\overline{x})$, provided that $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$ and that every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of at most N elements. To this end, let $\mathcal{B}$ be an arbitrary σ-structure from $\mathfrak{D}$ and let $\overline{b} \in B^n$.

If $\mathcal{B} \models \psi[\overline{b}]$, then there is a tuple $(\mathcal{A}, \overline{a}) \in \mathfrak{K}$ such that $\mathcal{B} \models \gamma_{(\mathcal{A},\overline{a})}[\overline{b}]$. Due to the Chandra-Merlin theorem (that is, Theorem 6.3.3 above), there is a homomorphism h from $\mathcal{A}$ to $\mathcal{B}$ with $\overline{b} = h(\overline{a})$. As $\mathcal{A} \in \mathfrak{D}$ and $\mathcal{A} \models \varphi[\overline{a}]$ by construction of $\mathfrak{K}$, and since $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, we obtain that $\mathcal{B} \models \varphi[\overline{b}]$.

Now suppose that $\mathcal{B} \models \varphi[\overline{b}]$. As $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$ it is, in particular, also preserved under extensions on $\mathfrak{D}$. Thus, $\mathcal{B}$ is either an extension of a structure $\mathcal{A} \in \mathfrak{D}$ such that $(\mathcal{A}, \overline{b})$ is a $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ or $(\mathcal{B}, \overline{b})$ itself is a $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$. In the latter case, we let $\mathcal{A} \coloneqq \mathcal{B}$. By assumption, N is an upper bound on the size of the universe of $\mathcal{A}$. Thus, by choice of $\mathfrak{K}$, the set $\mathfrak{K}$ contains a tuple $(\mathcal{A}', \overline{a}')$ for which there is an isomorphism $h\colon A' \to A$ from $\mathcal{A}'$ to $\mathcal{A}$ with $\overline{b} = h(\overline{a}')$. Since, more general, h is a homomorphism from $\mathcal{A}'$ to $\mathcal{B}$, we obtain from Theorem 6.3.3 that $\mathcal{B} \models \gamma_{(\mathcal{A}', \overline{a}')}[\overline{b}]$ and thus, since $(\mathcal{A}', \overline{a}') \in \mathfrak{K}$, also $\mathcal{B} \models \psi[\overline{b}]$.

In summary, this shows that $\psi(\overline{x})$ is $\mathfrak{D}$-equivalent to $\varphi(\overline{x})$.

Size and time complexity. The cardinality of the set $\mathfrak{K}$ is bounded by the number of all tuples $(\mathcal{A}, \overline{a})$ where $\mathcal{A}$ is a σ-structure with universe $[1, M]$ for an $M \leq N$ and where $\overline{a} \in A^n$, and thus by

$$\sum_{M=1}^{N} M^n \cdot 2^{\max\{2,M\}^{||\sigma||}} \;\leq\; N^{n+1} \cdot 2^{N^{||\sigma||}} \;\in\; 2^{(n+1) \cdot N^{\mathcal{O}(||\sigma||)}}. \tag{1}$$

Furthermore, for each tuple $(\mathcal{A}, \overline{a}) \in \mathfrak{K}$, the canonical conjunctive query $\gamma_{(\mathcal{A}, \overline{a})}(\overline{x})$ can be constructed in time

$$\mathcal{O}(n) + N^{\mathcal{O}(||\sigma||)}. \tag{2}$$

Hence, using Estimate (1) and Estimate (2), the size of $\psi(\overline{x})$ is also in

$$2^{(n+1) \cdot N^{\mathcal{O}(||\sigma||)}}.$$

Let us now turn to the algorithm's Step (1) and the analysis of its time complexity. To compute the set $\mathfrak{K}$, the algorithm enumerates all σ-structures $\mathcal{A}$ whose universe is the set $[1, M]$ for some $M \in [1, N]$ and checks whether $\mathcal{A} \in \mathfrak{C}'$. If this is the case, the algorithm enumerates all tuples $\overline{a} \in A^n$ and decides whether also $\mathcal{A} \models \varphi[\overline{a}]$.

By assumption, it can be decided in time $t(||\sigma|| + ||\mathcal{A}||)$, respectively in time $t(N^{\mathcal{O}(||\sigma||)})$, whether $\mathcal{A} \in \mathfrak{C}'$. For an ultimately periodic logic L, a naive model-checking algorithm can proceed in the same fashion as for the case of FO, that is, by recursion over the shape of φ and, for each ultimately periodic quantifier, interpreting the tuple of quantified variables by all possible tuples of elements of A with the same length. Thus, it takes time in $N^{||\varphi|| \cdot \mathcal{O}(||\sigma||)}$ to decide whether $\mathcal{A} \models \varphi[\overline{a}]$.

Using Estimate (1) on the cardinality of $\mathfrak{K}$ and recalling that $n+1 < ||\varphi||$, the entire computation of $\mathfrak{K}$ and ψ takes time in

$$\begin{aligned} & 2^{(n+1)\cdot N^{\mathcal{O}(||\sigma||)}} \cdot \Big(t(N^{\mathcal{O}(||\sigma||)}) + N^{\mathcal{O}(||\sigma||)\cdot||\varphi||}\Big) \\ \subseteq \;\; & 2^{||\varphi||\cdot N^{\mathcal{O}(||\sigma||)}} \cdot t(N^{\mathcal{O}(||\sigma||)}). \end{aligned}$$

This completes the proof of Lemma 6.3.2. □

Before combining Theorem 6.3.1 and Lemma 6.3.2 into a proof of Theorem 6.1.10, we recapitulate a proof of the Chandra-Merlin theorem, as stated in Theorem 6.3.3.

Proof of Theorem 6.3.3. Let σ be a relational signature, let $\mathcal{A}, \mathcal{B}$ be σ-structures, and let $\overline{a} = (a_1, \dots, a_n) \in A^n$ and $\overline{b} = (b_1, \dots, b_n) \in B^n$ be tuples of length $n \geq 0$. We assume that the universe of $\mathcal{A}$ is a subset of the natural numbers. Let $M := |A|$ and let $e_1, \dots, e_M$ with $e_1 < \cdots < e_M$ denote the elements of A. Furthermore, choose indices $j_1, \dots, j_n \in [1, M]$ such that $(a_1, \dots, a_n) = (e_{j_1}, \dots, e_{j_n})$.

We prove the two directions of the equivalence of Theorem 6.3.3.

For the "only if" direction, suppose that $\mathcal{B} \models \gamma_{(\mathcal{A},\overline{a})}[\overline{b}]$. Then, there are (not necessarily distinct) elements $c_1, \dots, c_M$ in B such that $\mathcal{B} \models \delta_{\mathcal{A}}[c_1, \dots, c_M]$.

Claim 1. *The function $h\colon A \to B$ with $h(e_i) = c_i$ for all $i \in [1, M]$ is a homomorphism from $\mathcal{A}$ to $\mathcal{B}$ such that $\overline{b} = h(\overline{a})$.*

Proof of Claim 1. By construction of the canonical conjunctive query $\gamma_{(\mathcal{A},\overline{a})}(\overline{x})$, $b_i = c_{j_i} = h(e_{j_i}) = h(a_i)$ for all $i \in [1, n]$. To show that h is indeed a homomorphism from $\mathcal{A}$ to $\mathcal{B}$, let R be a relation symbol from σ with arity $r \geq 1$, and suppose that, for indices $i_1, \dots, i_r$ from $[1, M]$, the tuple $(e_{i_1}, \dots, e_{i_r})$ belongs to the relation $R^{\mathcal{A}}$. Thus, the atomic formula $R(y_{i_1}, \dots, y_{i_r})$ occurs in the conjunction $\delta_{\mathcal{A}}(y_1, \dots, y_M)$. Since $\mathcal{B} \models \delta_{\mathcal{A}}[c_1, \dots, c_M]$ it follows that, in particular, $(c_{i_1}, \dots, c_{i_r}) = (h(e_{i_1}), \dots, h(e_{i_r}))$ belongs to the relation $R^{\mathcal{B}}$.

This completes the proof of Claim 1 and the "only if" direction of Theorem 6.3.3.

For the "if" direction, suppose that there is a homomorphism h from $\mathcal{A}$ to $\mathcal{B}$ where $\overline{b} = h(\overline{a})$. For each $i \in [1, M]$, let $c_i := h(e_i)$. Let $R(y_{i_1}, \dots, y_{i_r})$, for a relation symbol R from σ with arity $r \geq 1$ and indices $i_1, \dots, i_r \in [1, M]$, be an atomic formula from the conjunction $\delta_{\mathcal{A}}(y_1, \dots, y_M)$. By construction of $\delta_{\mathcal{A}}(y_1, \dots, y_m)$, we know that the tuple $(e_{i_1}, \dots, e_{i_r})$ belongs to the relation $R^{\mathcal{A}}$. Since h is a homomorphism from $\mathcal{A}$ to $\mathcal{B}$, it follows that the tuple $(h(e_{i_1}), \ldots, h(e_{i_r})) = (c_{i_1}, \ldots, c_{i_r})$ belongs to the relation $R^{\mathcal{B}}$. Hence, $\mathcal{B} \models \delta_{\mathcal{A}}[c_1, \ldots, c_M]$. Furthermore, by choice of $c_1, \ldots, c_M$ and the assumption on the homomorphism h, we have that $b_i = h(a_i) = h(e_{j_i}) = c_{j_i}$ for each $i \in [1, n]$. Altogether, we can conclude that $\mathcal{B} \models \gamma_{(\mathcal{A},\overline{a})}[\overline{b}]$ when interpreting the quantified variables $y_1, \ldots, y_M$ in $\gamma_{(\mathcal{A},\overline{a})}(\overline{x})$ by the elements $c_1, \ldots, c_M$ from B.

This completes the proof of Theorem 6.3.3. □

Theorem 6.1.10 is now obtained by a straightforward combination of Theorem 6.3.1 and Lemma 6.3.2.

Proof of Theorem 6.1.10. Let $\mathfrak{C}'$ be a class of structures (of arbitrary relational signatures) that is closed under disjoint unions and induced substructures and decidable in time $t(n)$ for some function $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$. Furthermore, let $d \geq 2$ a degree bound and denote by $\mathfrak{C}'_d$ the class of all d-bounded structures in $\mathfrak{C}'$.

For a structure $\mathcal{A}$ of some relational signature, it can be decided in time $d \cdot \mathcal{O}(||\mathcal{A}||^2)$ whether $\mathcal{A}$ has degree $\leq d$: For this, an adjacency list representation of $\mathcal{A}$'s Gaifman-graph $\mathcal{G}_{\mathcal{A}}$ is computed. For each tuple of length $r \geq 1$ in every relation of $\mathcal{A}$, less than r^2 edges have to be added to $\mathcal{G}_{\mathcal{A}}$. Since the adjacency list for each element of $\mathcal{A}$ only has to be computed for $\leq d$ entries, each edge can be added in time $\mathcal{O}(d)$.

Thus, whether a structure $\mathcal{A}$ belongs to $\mathfrak{C}'_d$ can be decided in time

$$t'_d(||\mathcal{A}||) \;\coloneqq\; t(||\mathcal{A}||) + d \cdot \mathcal{O}(||\mathcal{A}||^2).$$

Clearly, the algorithm of Lemma 6.3.2 is uniform in the degree bound d, when choosing $\mathfrak{C}'_d$ as the underlying class of structures. That is, we can consider d as an input to the algorithm.

Let σ be a relational signature and let $\mathfrak{D}$ denote the class of all σ-structures from $\mathfrak{C}'_d$. Furthermore, let $\varphi(\overline{x})$ be a formula from FO+unM$[\sigma]$ with quantifier rank $q \geq 0$ and $n \geq 0$ free variables that is preserved under homomorphisms on $\mathfrak{D}$.

The algorithm proceeds in the following steps:

(Step 1) Compute the upper bound

$$N \;\coloneqq\; N^{d,||\sigma||}(n,q) \quad\in\quad (n{+}1) \cdot S^{d,||\sigma||}(2 \cdot 4^q)$$

on the size of $\mathfrak{D}$-minimal models of $\varphi(\overline{x})$, obtained from Theorem 6.3.1. Observe that $N \geq 2$.

(Step 2) Using this upper bound, the algorithm of Lemma 6.3.2 constructs an existential-positive formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ that is $\mathfrak{D}$-equivalent to $\varphi(\overline{x})$. This takes time in

$$\begin{aligned} & 2^{||\varphi||\cdot((n+1)\cdot S^{d,||\sigma||}(2\cdot 4^q))^{\mathcal{O}(||\sigma||)}} \cdot t(((n+1)\cdot S^{d,||\sigma||}(2\cdot 4^q))^{\mathcal{O}(||\sigma||)}) \\ \subseteq\ & 2^{||\varphi||\cdot(n+1)^{\mathcal{O}(||\sigma||)}\cdot S^{d,||\sigma||}(2\cdot 4^q)} \cdot t((n+1)^{\mathcal{O}(||\sigma||)}\cdot S^{d,||\sigma||}(2\cdot 4^q)) \\ \subseteq\ & 2^{||\varphi||\cdot(n+1)^{\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}} \cdot t((n+1)^{\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}) \end{aligned}$$

Furthermore, the constructed existential-positive formula $\psi(\overline{x})$ has size in

$$2^{(n+1)\cdot((n+1)\cdot S^{d,||\sigma||}(2\cdot 4^q))^{\mathcal{O}(||\sigma||)}} \quad\subseteq\quad 2^{(n+1)^{\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}}.$$

This completes the proof of Theorem 6.1.10. ☐

6.4 Closure Properties

Theorem 6.1.7 and Theorem 6.1.10 require that the considered classes be closed under disjoint unions and induced substructures. This section provides examples which show that these closure properties are indeed necessary.

Both examples use graphs that are directed paths where some endpoints are coloured green. More precisely, these are structures $\mathcal{P}$ over the signature $\sigma := (E, G)$, where G is an additional unary relation symbol, whose (E)-reduct is a graph which solely consists of nodes on a directed path. The nodes in the relation $G^{\mathcal{P}}$ are called "green nodes". Moreover, a node is a *left endpoint* or a *right endpoint* if it has no ingoing or no outgoing edge, respectively. An *endpoint* is either a left or a right endpoint. For $n \geq 1$, a directed path on n nodes where exactly the endpoints are coloured green will be denoted by $\mathcal{P}_n$ and a directed path on $2n+1$ nodes where just the central node is coloured green will be denoted by $\mathcal{C}_n$.

Theorem 6.4.1. *There is a class $\mathfrak{C}'$ of σ-structures of degree at most 2 that is closed under substructures but not under disjoint unions, and there is a sentence φ in $\mathsf{FO}[\sigma]$ that is preserved under extensions and homomorphisms on $\mathfrak{C}'$, but that has no $\mathfrak{C}'$-equivalent existential sentence in $\mathsf{FO}[\sigma]$.*

Proof. Let $\mathfrak{C}'$ be the class that contains precisely the σ-structures for which there is an $n \geq 1$ such that the structure is isomorphic to a substructure of $\mathcal{P}_n$. By construction, $\mathfrak{C}'$ is closed under substructures. It is not closed under disjoint unions, since e. g., the disjoint union of two copies of $\mathcal{P}_n$, for some $n \geq 1$, is not a substructure of $\mathcal{P}_m$ for any $m \geq 1$.

There is an obvious sentence φ in $\mathsf{FO}[\sigma]$ that is satisfied by a σ-structure $\mathcal{A}$ if and only if $|A| \geq 3$ and all endpoints of $\mathcal{A}$ are green. The models of φ that belong to $\mathfrak{C}'$ are exactly the structures that are isomorphic to $\mathcal{P}_n$ for some $n \geq 3$, because each structure $\mathcal{A}$ with $|A| \geq 3$ that is isomorphic to a proper substructure of some $\mathcal{P}_n$ contains an endpoint that is not green. The sentence φ is preserved under homomorphisms (and hence also under extensions) on $\mathfrak{C}'$ for the reason that the only structure in $\mathfrak{C}'$ to which there is a homomorphism from $\mathcal{P}_n$ is $\mathcal{P}_n$ itself.

It remains to show that on $\mathfrak{C}'$ the formula φ is not equivalent to an existential sentence. Assume towards a contradiction that φ is $\mathfrak{C}'$-equivalent to an existential sentence $\psi := \exists x_1 \cdots \exists x_k \, \gamma(x_1, \ldots, x_k)$, where $k \geq 1$ and where γ is quantifier-free. In particular, $\mathcal{P}_{k+3} \models \psi$ so that there are nodes $a_1, \ldots, a_k$ in P_{k+3} for which $\mathcal{P}_{k+3} \models \gamma[a_1, \ldots, a_k]$. Let $\mathcal{P}$ be the substructure of $\mathcal{P}_{k+3}$ induced by $\{a_1, \ldots, a_k\}$. Clearly, $\mathcal{P} \models \gamma[a_1, \ldots, a_k]$ and so $\mathcal{P} \models \psi$. On the other hand, $\mathcal{P}$ contains at least one endpoint that is not coloured green. Therefore, $\mathcal{P} \not\models \varphi$. This contradicts our assumption that φ and ψ are equivalent. □

Theorem 6.4.2. *There is a class $\mathfrak{C}''$ of σ-structures of degree at most 2 that is closed under disjoint unions but not under induced substructures, and there is a sentence φ in $\mathsf{FO}[\sigma]$ that is preserved under extensions and homomorphisms on $\mathfrak{C}''$, but that has no $\mathfrak{C}''$-equivalent existential sentence in $\mathsf{FO}[\sigma]$.*

Proof. Let $\mathfrak{C}''$ be the class of all σ-structures that are disjoint unions of structures that are isomorphic to $\mathcal{P}_n$ or $\mathcal{C}_m$, for $n, m \geq 1$. By construction, $\mathfrak{C}''$ is closed under disjoint unions. It is not closed under induced substructures, since, e. g., $\mathcal{P}_3$ has an isolated node that is not coloured green as an induced substructure, but such graphs do not belong to $\mathfrak{C}''$.

There is an obvious sentence φ in $\mathsf{FO}[\sigma]$ that is satisfied by a σ-structure $\mathcal{A}$ if and only if $|A| \geq 2$ and $\mathcal{A}$ contains a green endpoint. A structure belonging to $\mathfrak{C}''$ satisfies φ if and only if it contains a copy of $\mathcal{P}_n$ for some $n \geq 2$, since no $\mathcal{C}_n$ for any $n \geq 1$ contains a green endpoint. The sentence φ is preserved under homomorphisms (and hence also under extensions) on $\mathfrak{C}''$ because there is no homomorphism from $\mathcal{P}_n$ with $n \geq 2$ to $\mathcal{C}_m$ for any $m \geq 1$ whatsoever, due to the two green endpoints.

It remains to show that φ is not $\mathfrak{C}''$-equivalent to an existential sentence. Assume to the contrary that φ is $\mathfrak{C}''$-equivalent to an existential sentence ψ of the shape $\exists x_1 \cdots \exists x_k\, \gamma(x_1, \ldots, x_k)$, where $k \geq 1$ and where γ is quantifier-free. Then $\mathcal{P}_{k+1} \models \psi$, which implies that there are nodes $a_1, \ldots, a_k$ in P_{k+1} for which $\mathcal{P}_{k+1} \models \gamma[a_1, \ldots, a_k]$. Let $M \coloneqq \{a_1, \ldots, a_k\}$. We partition M into sets L, R, where L is the (possibly empty) set of all nodes nodes from M that belong to the connected component, in $\mathcal{P}_{k+1}[M]$, of the left endpoint of $\mathcal{P}_{k+1}$, and let $R \coloneqq M \setminus L$. Clearly, L and R are disconnected in $\mathcal{P}_{k+1}[M]$ and, in particular, the set L can not contain the right endpoint of $\mathcal{P}_{k+1}$.

Suppose that L is empty and thus, $R = M$. There is a set $M' \subseteq C_k$ of nodes "left of" the central green node in $\mathcal{C}_k$ such that $\mathcal{C}_k[M'] \cong \mathcal{P}_{k+1}[M]$. Hence, $\mathcal{C}_k \models \psi$. But clearly $\mathcal{C}_k[M'] \not\models \varphi$. This is a contradiction.

In the case that L is not empty, the path $\mathcal{C}_k$ contains induced substructures that are isomorphic to $\mathcal{P}_{k+1}[L]$ and $\mathcal{P}_{k+1}[R]$, respectively ("right of" and "left of" the central green node). Let $\mathcal{A}$ be the disjoint union of two copies $\mathcal{A}_1$ and $\mathcal{A}_2$ of $\mathcal{C}_k$. We map the nodes in L and R to the corresponding nodes of $\mathcal{A}_1$ and $\mathcal{A}_2$, respectively. Now let M' be the image of M under this mapping. It is easy to verify that $\mathcal{A}[M'] \cong \mathcal{P}_{k+1}[M]$. Hence, $\mathcal{A} \models \psi$. But clearly $\mathcal{A} \not\models \varphi$. This is a contradiction. $\square$

6.5 Conclusion

In this chapter, we have developed elementary algorithms that construct, on input of a formula from $\mathsf{FO{+}unM}[\sigma]$, for some relational signature σ, that is preserved under extensions (homomorphisms) on the class $\mathfrak{C}^{d,\sigma}$ of d-bounded σ-structures, a d-equivalent existential (existential-positive) $\mathsf{FO}[\sigma]$-formula.

For preservation under extensions, the algorithm has actually 5-fold (3-fold) exponential time complexity in the size of the input formula for degree bounds $d \geq 3$ ($d = 2$). For preservation under homomorphisms, its time complexity is 4-fold (3-fold) exponential.

Note that both results do not only hold for the class $\mathfrak{C}^{d,\sigma}$ of all d-bounded σ-structures but, more generally, for classes of d-bounded σ-structures that are closed under disjoint unions and induced substructures (and, for preservation under homomorphisms, decidable in 1-fold exponential time). In this direction, we have also shown that the mentioned closure properties are not just required by our specific proofs but are indeed necessary to ensure the existence of corresponding existential, and thus, existential-positive sentences.

Both proofs consisted of two basic steps: In the first step, an upper bound on the size of $\mathfrak{C}^{d,\sigma}$-minimal models for the input formula was found. For the case of preservation under extensions, we applied a novel iterative construction using the locality theorem for $\mathsf{FO}+\mathrm{unM}$, stated in Section 3.3. For the case of preservation under homomorphisms, a construction of Ajtai and Gurevich [AG94] was adapted to this locality theorem. In the second step, the upper bound on the size of $\mathfrak{C}^{d,\sigma}$-minimal models is used for the construction of the actual existential or existential-positive sentence. For preservation under extensions, we extended a method from [DGKS07], while for preservation under homomorphisms, the construction is based on the Chandra-Merlin theorem [CM77].

For both algorithms, Section 9.6 provides non-matching 3-fold exponential lower bounds for degree bound $d = 3$.

In Section 7.5, we will extend the above mentioned algorithms to formulae from $\mathsf{FO}+\mathrm{unM}_{\mathrm{tpl}}$ and, in Section 8.6, finally to formulae from arbitrary ultimately periodic logics.

7 Tuple-Counting Quantifiers

This chapter extends the results of the previous chapters concerning Hanf normal form, Feferman-Vaught decompositions, and preservation theorems, to formulae with modulo-counting and threshold-counting quantifiers that may not only count single elements, but tuples of elements. Towards this aim it is shown, using a well-known construction (see [Str94]), how formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ can be turned into equivalent formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ with the same quantifier rank, threshold, and maximum period.

This transformation is then used in algorithms that compute, on classes of structures of bounded degree and for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$, Hanf normal form and existential or existential-positive formulae (in the latter two cases, provided that the input formula is preserved under extensions or homomorphisms on the corresponding class, respectively).

For Feferman-Vaught decompositions, we obtain analogous results. In particular, tuple-counting quantifiers allow here the construction of decompositions obtained from transductions on disjoint sums and, in particular, decompositions with respect to direct products of structures for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ and, moreover, from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$. In Chapter 5, this was only possible for FO.

7.1 Introduction

Recall that a formula of the shape

$$\mathsf{Q}(y_1, \ldots, y_m)\, \varphi(\overline{y}),$$

with $\mathsf{Q} \subseteq \mathbb{N}$ and a tuple $\overline{y} = (y_1, \ldots, y_m)$ of $m \geq 1$ pairwise distinct variables, is satisfied by a structure $\mathcal{A}$ of suitable signature if and only if

$$|\{\overline{a} \in A^n \,:\, \mathcal{A} \models \varphi[\overline{a}]\}| \;\in\; \mathsf{Q}.$$

In this chapter we want to express such formulae by formulae which only make use of counting quantifiers that count single elements, that is, where only $m = 1$

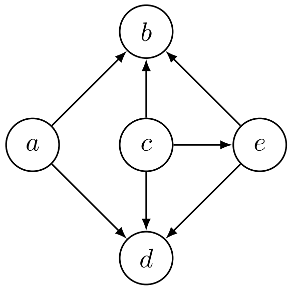

Figure 7.1 The graph $\mathcal{A}$ of example Example 7.1.1.

is allowed. Clearly, the formula $\exists(y_1, \ldots, y_m)\,\varphi$ is equivalent to the formula $\exists y_1 \cdots \exists y_m\,\varphi$. The following example shows that this does not carrys over to other quantifiers:

Example 7.1.1. The sentence

$$\exists^{\equiv 0 \bmod 2}(y_1, y_2)\, E(y_1, y_2) \tag{7.1}$$

over the signature (E) expresses that the number of directed edges in a graph is even. In particular, the graph $\mathcal{A}$ depicted in Figure 7.1 does not satisfy the sentence. The sentence

$$\exists^{\equiv 0 \bmod 2} y_1\, \exists^{\equiv 0 \bmod 2} y_2\, E(y_1, y_2),$$

however, is satisfied by $\mathcal{A}$. On the other hand, it can be straightforwardly verified that Sentence (7.1) is equivalent to the sentence

$$\exists^{\equiv 0 \bmod 2} y_1\, \exists^{\equiv 1 \bmod 2} y_2\, E(y_1, y_2), \tag{7.2}$$

which expresses that there is an even number of nodes y_1 that have an edge to an odd number of nodes y_2. In particular, whether a graph has an even or odd number of directed edges does not depends on the number of nodes y_1 that have an edge to an even number of nodes y_2.

In the subsequent Section 7.2 we will generalise the observation which inspired Sentence (7.2) to modulo-counting quantifiers of arbitrary period and remainder and threshold-counting quantifiers that count tuples of arbitrary finite length. This will lead to an algorithm which turns arbitrary formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ into equivalent formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$.

In the remaining sections of this chapter, we will generalise the results of Chapter 3, Chapter 5, and Chapter 6 to formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$. The corresponding proofs will be straightforward and rely on the algorithm provided in Section 7.2 and the observation, that the transformation performed by this algorithm does not change the threshold or the periods of the quantifiers in the transformed formula.

7.2 Resolving Tuple-Counting Quantifiers

In this section, it is shown how formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ can be turned into equivalent formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$, that is, into formulae whose quantifiers only count single elements of structures.

The main result of this section is stated in the following theorem. Its proof is based on a construction described in [Str94, p. 164], which generalises the idea used in Sentence (7.2).

Theorem 7.2.1. *There is an algorithm which, on input of a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$ with $D \subseteq D_{\mathrm{all}}$ and σ being a relational signature, computes a formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ that is equivalent to $\varphi(\overline{x})$ and that has the same threshold and quantifier rank as $\varphi(\overline{x})$.*

Furthermore, the algorithm computes $\psi(\overline{x})$ in time

$$\mathcal{O}(||\varphi||) \cdot 2^{\mathcal{O}(q)\cdot(\log\max\{T+1,P\})^2},$$

where $T, P, q \geq 0$ are the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$, respectively. In particular, the constants suppressed by the $\mathcal{O}$-notation do not depend on the signature σ.

The proof of Theorem 7.2.1 proceeds by an induction on the shape of the input formula, which can be found at the end of this section. The crucial part of this induction is the handling of tuple-counting quantifiers, which is provided by the following Lemma 7.2.2 and Lemma 7.2.3.

Lemma 7.2.2 describes the handling of modulo-counting quantifiers.

Lemma 7.2.2. *Let σ be a relational signature, let $D \subseteq D_{\mathrm{all}}$, and let $m \geq 2$. For every formula*

$$\varphi(\overline{x}) \quad := \quad \exists^{\equiv k \bmod p}\overline{y}\,\gamma(\overline{x},\overline{y})$$

from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$, where $p \geq 2$, $k \in [0,p)$, $\overline{y}$ is a tuple of m pairwise distinct variables, and $\gamma(\overline{x},\overline{y})$ is a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$, there is a formula $\psi(\overline{x})$ in $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$ of dimension $m-1$ that is equivalent to $\varphi(\overline{x})$.

The formula $\psi(\overline{x})$ *has the same threshold and the same quantifier rank as* $\varphi(\overline{x})$ *and, moreover,* $\psi(\overline{x})$ *is a Boolean combination of formulae of the shape*

$$\exists^{\equiv j \bmod p}(y_1, \ldots, y_{m-1})\, \gamma'(\overline{x}, y_1, \ldots, y_{m-1}) \tag{7.3}$$

with $j \in [0, p)$ *and where* $\gamma'(\overline{x}, y_1, \ldots, y_{m-1})$ *is some formula from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$.

Furthermore, there is an algorithm that computes $\psi(\overline{x})$ *on input of* $\varphi(\overline{x})$ *in time*

$$||\varphi|| \cdot 2^{\mathcal{O}((\log p)^2)},$$

where the constant suppressed by the $\mathcal{O}$*-notation does not depend on the signature* σ*.*

Lemma 7.2.2 describes the handling of threshold-counting quantifiers.

Lemma 7.2.3. *Let* σ *be a relational signature, let* $D \subseteq D_{\mathrm{all}}$*, and let* $m \geq 2$*. For every formula*

$$\varphi(\overline{x}) \;\coloneqq\; \exists^{>k}\overline{y}\, \gamma(\overline{x}, \overline{y}),$$

where $k \geq 1$*,* $\overline{y}$ *is a tuple of* m *pairwise distinct variables, and* $\gamma(\overline{x}, \overline{y})$ *is a formula from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$*, there is a formula* $\psi(\overline{x})$ *in* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$ *of dimension* $m-1$ *that is equivalent to* $\varphi(\overline{x})$

The formula $\psi(\overline{x})$ *has the same threshold and the same quantifier rank as* $\varphi(\overline{x})$ *and, moreover,* $\psi(\overline{x})$ *is a Boolean combination of formulae from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ *and formulae of the shape*

$$\exists^{>j}(y_1, \ldots, y_m)\, \gamma'(\overline{x}, y_1, \ldots, y_{m-1}) \tag{7.4}$$

with $j \in [0, k]$ *and* $\gamma'(\overline{x}, y_1, \ldots, y_{m-1})$ *a formula from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$.

Furthermore, there is an algorithm that computes $\psi(\overline{x})$ *on input of* $\varphi(\overline{x})$ *in time*

$$||\varphi|| \cdot 2^{\mathcal{O}((\log(k+1))^2)},$$

where the constant suppressed by the $\mathcal{O}$*-notation does not depend on the signature* σ*.*

In the proofs of both lemmas, we generalise the idea of Sentence (7.2) in Example 7.1.1 to turn a formula of the shape

$$\varphi(\overline{x}) \;\coloneqq\; \mathsf{Q}\overline{y}\, \gamma(\overline{x}, \overline{y}),$$

where Q is either a modulo-counting quantifier $\exists^{\equiv k \bmod p}$ or a threshold-counting quantifier $\exists^{>k}$, where $\overline{x}, \overline{y}$ are tuples of $n \geq 0$ and $m \geq 2$ pairwise distinct variables, respectively, and where $\gamma(\overline{x}, \overline{y})$ is a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ for a set $D \subseteq D_{\mathrm{all}}$, into an equivalent formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$ of dimension $m-1$. For each σ-structure $\mathcal{A}$ and every tuple $\overline{a} \in A^n$, we let

$$W^{\varphi}[\mathcal{A}, \overline{a}] \;\coloneqq\; \{\overline{b} \in A^m \,:\, \mathcal{A} \models \gamma[\overline{a}, \overline{b}]\},$$

denote the *set of witnesses* of the quantifier Q in respect to the interpretation $(\mathcal{A}, \overline{a})$ for $\varphi(\overline{x})$. For each tuple $\overline{b} \in A^{m-1}$, we furthermore let

$$W^{\varphi}[\mathcal{A}, \overline{a}, \overline{b}] \;\coloneqq\; \{b \in A \,:\, \mathcal{A} \models \gamma[\overline{a}, \overline{b}, b]\}.$$

Example 7.2.4. For the sentence φ from (7.1), we have $n = 0$. Thus, for the graph $\mathcal{A}$ of Figure 7.1, we have $W^{\varphi}[\mathcal{A}, (), c] = \{b, d, e\}$.

Proof of Lemma 7.2.2. Let σ be a relational signature, let $D \subseteq D_{\mathrm{all}}$, and let $m \geq 2$. Furthermore, let $\varphi(\overline{x}) \coloneqq \exists^{\equiv k \bmod p}\overline{y}\,\gamma(\overline{x}, \overline{y})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$ where $p \geq 2$, $k \in [0, p)$, $|\overline{y}| = m$, and $\gamma(\overline{x}, \overline{y})$ is a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$.

For each σ-structure $\mathcal{A}$ and every tuple $\overline{a} \in A^n$, let

$$W^{\varphi}_j[\mathcal{A}, \overline{a}] \;\coloneqq \{\, \overline{b} \in A^{m-1} \colon |W^{\varphi}[\mathcal{A}, \overline{a}, \overline{b}]| \;\equiv\; j \mod p \,\}$$

for all $j \in [1, p)$. Clearly, the sets $W^{\varphi}_j[\mathcal{A}, \overline{a}]$ for all $j \in [1, p)$ are pairwise disjoint and, moreover,

$$\sum_{j=1}^{p-1} |W^{\varphi}_j[\mathcal{A}, \overline{a}]| \cdot j \;\equiv\; |W^{\varphi}[\mathcal{A}, \overline{a}]| \mod p. \tag{1}$$

Example 7.2.5. Continuing Example 7.2.4, we have $W^{\varphi}_0[\mathcal{A}, ()] = \{a, b, d, e\}$ and $W^{\varphi}_1[\mathcal{A}, ()] = \{c\}$ for the sentence φ from (7.1) and the graph $\mathcal{A}$ of Figure 7.1.

In the following, we define for each $i \in [0, p)$ and $j \in [1, p)$ a formula $\delta_j^{\equiv i \bmod p}(\overline{x})$, such that for each σ-structure $\mathcal{A}$ and every $\overline{a} \in A^n$,

$$\mathcal{A} \;\models\; \delta_j^{\equiv i \bmod p}[\overline{a}] \quad \text{iff} \quad |W^{\varphi}_j[\mathcal{A}, \overline{a}]| \cdot j \;\equiv\; i \mod p. \tag{2}$$

For each $\ell \in [0, p)$, we let

$$\varepsilon_j^{\equiv \ell \bmod p}(\overline{x}) \;\coloneqq\; \exists^{\equiv \ell \bmod p}(y_1, \ldots, y_{m-1})\, \exists^{\equiv j \bmod p} y_m\, \gamma(\overline{x}, \overline{y}).$$

Note that $\epsilon_j^{\equiv \ell \bmod p}(\overline{x})$ is of Shape (7.3) and of size $\mathcal{O}(||\varphi||)$.

We now let L be the set of all $\ell \in [0, p)$ such that $\ell \cdot j$ is congruent to i modulo p. If L is non-empty, we choose $\delta_j^{\equiv i \bmod p}(\overline{x})$ as the formula

$$\bigvee_{\ell \in L} \varepsilon_j^{\equiv \ell \bmod p}(\overline{x})$$

Note that in this case, $\delta_j^{\equiv i \bmod p}(\overline{x})$ is a disjunction of formulae of Shape (7.3) of size $p \cdot \mathcal{O}(||\varphi||)$. Otherwise, that is, if L is the empty set, we let $\delta_j^{\equiv i \bmod p}(\overline{x})$ be the unsatisfiable formula

$$\varepsilon_j^{\equiv 0 \bmod p}(\overline{x}) \ \wedge \ \neg\varepsilon_j^{\equiv 0 \bmod p}(\overline{x})$$

which is a Boolean combination of formulae of Shape (7.3) of size $\mathcal{O}(||\varphi||)$.

Now, $\psi(\overline{x})$ *could* be chosen as the formula

$$\bigvee_{f \in F} \bigwedge_{j=1}^{p-1} \delta_j^{\equiv f(j) \bmod p}(\overline{x}) \tag{3}$$

where F is the set of all functions $f\colon [1, p) \to [0, p)$ such that

$$\sum_{j=1}^{p-1} f(j) \ \equiv \ k \mod p.$$

To see this, consider a σ-structure $\mathcal{A}$ and a tuple $\overline{a} \in A^n$. Suppose first that $\mathcal{A} \models \varphi[\overline{a}]$, that is, $|W^\varphi[\mathcal{A}, \overline{a}]|$ is congruent k modulo p. Thus, by Congruence (1), there is a function $f \in F$ such that $|W_j^\varphi[\mathcal{A}, \overline{a}]| \cdot j$ is congruent to $f(j)$ for each $j \in [1, p)$. Hence, it follows from Equivalence (2) that $(\mathcal{A}, \overline{a})$ satisfies Formula (3).

For the other direction, suppose that $(\mathcal{A}, \overline{a})$ satisfies Formula (3). Then, there is a function $f \in F$ such that $|W_j^\varphi[\mathcal{A}, \overline{a}]| \cdot j$ is congruent to $f(j)$ for each $j \in [1, p)$ and thus, by definition of f and Congruence (1), $|W^\varphi[\mathcal{A}, \overline{a}]|$ is congruent k modulo p. It follows, that $\mathcal{A} \models \varphi[\overline{a}]$.

However, Formula (3) has size in $p^{p-1} \cdot p \cdot \mathcal{O}(||\varphi||)$ and thus grows exponentially with the period p. To obtain an equivalent formula that only grows polynomially with p, we use Lemma 2.9.2 and let

$$\psi(\overline{x}) \ := \langle \delta_j^{\equiv i \bmod p} \rangle_{[1,p)}^{\equiv k \bmod p}(\overline{x}).$$

Note that, in particular, $\psi(\overline{x})$ is a Boolean combination of formulae $\delta_j^{\equiv i \bmod p}(\overline{x})$ with $i \in [0, p)$ and $j \in [1, p)$.

Time complexity. For each $i \in [0,p)$ and $j \in [1,p)$, the formula $\delta_j^{\equiv i \bmod p}(\overline{x})$ has size in $p \cdot \mathcal{O}(||\varphi||)$. Thus, by Lemma 2.9.2, the construction of $\psi(\overline{x})$ takes time in

$$p \cdot \mathcal{O}(||\varphi||) \cdot (2p)^{\lceil \log p \rceil + 1} \quad \subseteq \quad ||\varphi|| \cdot 2^{\mathcal{O}((\log p)^2)}.$$

This completes the proof of Lemma 7.2.2. □

Proof of Lemma 7.2.3. Let σ be a relational signature and let $D \subseteq D_{\text{all}}$. Let $k \geq 1$, let $\overline{y}$ be a tuple of pairwise distinct variables of length $m \geq 2$, and let $\varphi(\overline{x}) := \exists^{>k}\overline{y}\,\gamma(\overline{x},\overline{y})$ with a formula $\gamma(\overline{x},\overline{y})$ from $\mathsf{FO}{+}\mathrm{unM}(D)[\sigma]$.

We proceed in a similar fashion as in the proof of Lemma 7.2.2. For each σ-structure $\mathcal{A}$ and every tuple $\overline{a} \in A^n$, let

$$V_j^{\varphi}[\mathcal{A},\overline{a}] \;:=\; \{\, \overline{b} \in A^{m-1} \colon |W^{\varphi}[\mathcal{A},\overline{a},\overline{b}]| \;=\; j \,\}$$

for all $j \in [1,k]$. Clearly, the sets $V_j^{\varphi}[\mathcal{A},\overline{a}]$ for all $j \in [1,k]$ are pairwise disjoint and $|W^{\varphi}[\mathcal{A},\overline{a}] > k$ if and only if one of the two following conditions holds:

(I) there is a $\overline{b} \in A^{m-1}$ such that $|W^{\varphi}[\mathcal{A},\overline{a},\overline{b}]| > k$

(II) $\displaystyle\sum_{j=1}^{k} |V_j^{\varphi}[\mathcal{A},\overline{a}]| \cdot j \;>\; k$

Condition (I) can be expressed by the formula

$$\psi_{\mathrm{I}}(\overline{x}) \;:=\; \exists y_1 \cdots \exists y_{m-1}\, \exists^{>k} y_m\, \gamma(\overline{x},\overline{y}).$$

In the following, we construct a formula $\psi_{\mathrm{II}}(\overline{x})$ that expresses Condition (II). For each $i \in [0,k]$ and $j \in [1,k]$, we let

$$\delta_j^{>i}(\overline{x}) \;:=\; \exists^{>\ell}(y_1,\ldots,y_{m-1})\, \exists^{=j} y_m\, \gamma(\overline{x},\overline{y})$$

where $\ell \in [0,k]$ is chosen minimal such that $(\ell{+}1) \cdot j > i$. Then, for each σ-structure $\mathcal{A}$ and every $\overline{a} \in A^n$,

$$\mathcal{A} \;\models\; \delta_j^{>i}[\overline{a}] \quad \text{iff} \quad |V_j^{\varphi}[\mathcal{A},\overline{a}]| \cdot j \;>\; i.$$

In a similar manner as in the proof of Lemma 7.2.2, one can verify that Condition (II) is expressed by the formula

$$\bigvee_{g \in G} \bigwedge_{\substack{j \in [1,k], \\ g(j) \geq 0}} \delta_j^{>i}(\overline{x})$$

where G is the set of all functions $g\colon [1,k] \to [-1,k]$ such that the sum of $g(j)+1$ for all $j \in [1,k]$ equals $k+1$. By Lemma 2.9.4, we can replace the latter formulae by the equivalent formula

$$\psi_{\mathrm{II}}(\overline{x}) \;\; := \;\; \langle \delta_j^{>i} \rangle_{[1,k]}^{>k}(\overline{x}),$$

where $\langle \delta_j^{>i} \rangle_{[1,k]}^{>k}(\overline{x})$ is a Boolean combination of formulae $\delta_j^{>i}(\overline{x})$ with $i \in [0,k]$ and $j \in [1,k]$.

Altogether, we can choose

$$\psi(\overline{x}) \;\; := \;\; \psi_{\mathrm{I}}(\overline{x}) \;\vee\; \psi_{\mathrm{II}}(\overline{x}).$$

Time complexity. The formula $\psi_{\mathrm{I}}(\overline{x})$ as well as each formula $\delta_j^{>i}(\overline{x})$ for $i \in [0,k]$ and $j \in [1,k]$ has size in $\mathcal{O}(||\varphi||)$. Thus, by Lemma 2.9.4, the construction of $\psi(\overline{x})$ takes time in

$$\mathcal{O}(||\varphi||) + \mathcal{O}(||\varphi||) \cdot (2k{+}2)^{\lceil \log k \rceil + 1} \quad \subseteq \quad ||\varphi|| \cdot 2^{\mathcal{O}((\log(k+1))^2)}.$$

This completes the proof of Lemma 7.2.3. □

We are now ready to prove Theorem 7.2.1 by using Lemma 7.2.2 and Lemma 7.2.3.

Proof of Theorem 7.2.1. Let σ be a relational signature, let $D \subseteq D_{\mathrm{all}}$, and let $\varphi(\overline{x})$ a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$. Furthermore, let $T, P, q \geq 0$ denote the threshold, the maximum period, and the quantifier rank of φ, respectively.

In the special case of a formula $\varphi(\overline{x})$ from $\mathsf{FO}_{\mathrm{tpl}}[\sigma]$, we replace each subformula of the shape $\exists(y_1, \ldots, y_m)\, \varphi'$ with $m \geq 2$ by the formula $\exists y_1 \cdots \exists y_m\, \varphi'$. This takes altogether time in $\mathcal{O}(||\varphi||)$.

Observe that otherwise, $T \geq 1$ or $P \geq 2$. In this case, the algorithm proceeds by an induction over the shape of $\varphi(\overline{x})$, where we show the following inductive invariant to hold for the constructed formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$:

Claim 1.

(a) *$\psi(\overline{x})$ is equivalent to $\varphi(\overline{x})$.*

(b) *$\psi(\overline{x})$ has the same threshold and quantifier rank as $\varphi(\overline{x})$.*

(c) *There are numbers $c, d \in \mathbb{N}_{\geq 1}$ (whose size is independent of $||\sigma||$), such that the algorithm terminates after at most*

$$c \cdot ||\varphi|| \cdot 2^{d \cdot q \cdot (\log \max\{T+1, P\})^2}$$

time steps.

If φ is a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$, there is nothing to do and we let $\psi \coloneqq \varphi$. Clearly, Claim 1 is satisfied.

Suppose that $\varphi(\overline{x})$ is a Boolean combination of formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$. If $\varphi = \neg\varphi'$, the algorithm computes a suitable formula ψ' from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ for φ' and outputs $\psi \coloneqq \neg\psi'$. If $\varphi = (\varphi' \vee \varphi'')$, the algorithm computes formulae ψ' and ψ'' from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ for φ' and φ'', respectively, and outputs the formula $\psi \coloneqq (\psi' \vee \psi'')$. It is straightforward to verify that Claim 1 is satisfied.

Suppose that $\varphi(\overline{x})$ has the shape $\mathsf{Q}\overline{y}\,\varphi'(\overline{x},\overline{y})$. Let $m \coloneqq |\overline{y}|$ and recall that φ' has quantifier rank $q - m$.

In a first step, the algorithm computes a formula $\psi'(\overline{x},\overline{y})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ for $\varphi'(\overline{x},\overline{y})$, such that the following holds:

(a') $\psi'(\overline{x})$ is equivalent to $\varphi'(\overline{x})$.

(b') $\psi'(\overline{x})$ has the same threshold and quantifier rank as $\varphi'(\overline{x})$.

(c') The algorithm took at most

$$c \cdot ||\varphi'|| \cdot 2^{d\cdot(q-m)\cdot(\log\max\{T+1,P\})^2} \tag{1}$$

time steps to construct $\psi'(\overline{x})$ from $\varphi'(\overline{x})$.

If $m = 1$, that is, $\overline{y}$ is a single variable y, then $\psi(\overline{y})$ can be chosen as $\mathsf{Q}y\,\psi'(\overline{x},\overline{y})$. For the following, we suppose that $m \geq 2$ and perform a case distinction by the shape of the quantifier Q.

(Case 1) *If $\mathsf{Q} = \exists^{\equiv k \bmod p}$ for a period $p \in [2,P]$ and $k \in [0,p)$*, the formula $\psi(\overline{x})$ is constructed by applying the algorithm of Lemma 7.2.2 to the formula $\exists^{\equiv k \bmod p}\overline{y}\,\psi'(\overline{x},\overline{y})$ and then to all subformulae of the resulting formula of Shape (7.3). This process has to be repeated $m-1$ times, until a formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ is reached that is equivalent to $\varphi(\overline{x})$ and has the same threshold and quantifier rank.

Thus, it follows from Lemma 7.2.2, that a constant $d \in \mathbb{N}_{\geq 1}$ can be chosen such that this process takes at most

$$||\psi'|| \cdot 2^{d\cdot(m-1)\cdot(\log p)^2} \quad \leq \quad ||\psi'|| \cdot 2^{d\cdot(m-1)\cdot(\log P)^2}$$

time steps.

(Case 2) *If $\mathsf{Q} = \exists^{>0} = \exists$*, the algorithm outputs $\psi(\overline{x}) \coloneqq \exists y_1 \cdots \exists y_m\,\psi'(\overline{x},\overline{y})$, where $(y_1,\ldots,y_m) = \overline{y}$.

(Case 3) *If* $\mathsf{Q} = \exists^{>k}$ *for some* $k \in [1, T]$, the formula $\psi(\overline{x})$ is constructed by applying the algorithm of Lemma 7.2.3 to the formula $\exists^{>k}\overline{y}\,\psi'$ and then to all subformulae of the resulting formula of Shape (7.4). This process has to be repeated $m-1$ times, until a formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{unM}(D)[\sigma]$ is reached that is equivalent to $\varphi(\overline{x})$ and has the same threshold and quantifier rank.

By Lemma 7.2.3, the constant $d \in \mathbb{N}_{\geq 1}$ can be chosen such that this takes at most

$$||\psi'|| \cdot 2^{d\cdot(m-1)\cdot(\log(k+1))^2} \quad \leq \quad ||\psi'|| \cdot 2^{d\cdot(m-1)\cdot(\log(T+1))^2}$$

time steps.

We have already seen that the constructed formula $\psi(\overline{x})$ satisfies Statement (a) and Statement (b) of Claim 1.

For Statement (c), note that Estimate (1) is also an upper bound on the size of $\psi'(\overline{x})$. Thus, $\psi(\overline{x})$ can be constructed in time

$$\begin{aligned} & 2^{d\cdot(m-1)\cdot(\log\max\{T+1,P\})^2} \cdot c \cdot ||\varphi'|| \cdot 2^{d\cdot(q-m)\cdot(\log\max\{T+1,P\})^2} \\ \leq \quad & c \cdot ||\varphi|| \cdot 2^{d\cdot q\cdot(\log\max\{T+1,P\})^2}. \end{aligned}$$

This completes the inductive construction of $\psi(\overline{x})$ which, by Statement (c) of Claim 1, altogether takes time in

$$\mathcal{O}(||\varphi||) \cdot 2^{\mathcal{O}(q)\cdot(\log\max\{T+1,P\})^2}.$$

Thus, the proof of Theorem 7.2.1 is completed. □

7.3 Hanf Normal Form

In this section, we use the construction of the previous section to extend the results of Chapter 3 from the logic $\mathsf{FO}{+}\mathrm{unM}$ to $\mathsf{FO}{+}\mathrm{unM}_{\mathrm{tpl}}$. The proofs are straightforward combinations of Theorem 7.2.1 and the corresponding theorem in Chapter 3.

7.3.1 Constructing Hanf Normal Form

This section generalises Theorem 3.2.1 to input formulae from $\mathsf{FO}{+}\mathrm{unM}_{\mathrm{tpl}}$, which can be stated as follows.

Theorem 7.3.1. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$,
- *a relational signature* σ, *and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$, *for a set* $D \subseteq D_{\mathrm{all}}$,

computes a HNF*-formula* $\psi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ *that is d-equivalent to* $\varphi(\overline{x})$.

Let $T, P, n, q \geq 0$ *be the threshold, the maximum period, the number of free variables, and the quantifier rank of* $\varphi(\overline{x})$, *respectively.*

Then, the computed formula $\psi(\overline{x})$ *has locality radius* $\leq 4^q$ *and threshold*

$$< \; T + (n{+}q) \cdot \nu_d(4^q).$$

Moreover, the algorithm constructs $\psi(\overline{x})$ *in time*

$$2^{\left(||\varphi|| \cdot 2^{q \cdot (\log \max\{T+1,P\})^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}.$$

Remark 7.3.2. In particular, the upper bounds on the locality radius and the threshold of the computed HNF-formula do not change in the generalisation of Theorem 3.2.1 from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ to $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$.

Furthermore, under the assumption that $||\sigma|| < ||\varphi||$, the algorithm also takes 3-fold exponential time in the size of $\varphi(\overline{x})$ for $d \geq 3$, and 2-fold exponential time in the size of $\varphi(\overline{x})$ for $d = 2$, since $T, P, q < ||\varphi||$.

Proof of Theorem 7.3.1. Let σ be a relational signature, let $D \subseteq D_{\mathrm{all}}$, and let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$. Furthermore, let $d \geq 2$ be a degree bound.

The algorithm proceeds in the following two steps:

(Step 1) The algorithm described in the proof of Theorem 7.2.1 constructs a formula $\tilde{\varphi}(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ that is equivalent to $\varphi(\overline{x})$. This takes time in

$$\mathcal{O}(||\varphi||) \cdot 2^{\mathcal{O}(q) \cdot (\log \max\{T+1,P\})^2}, \tag{1}$$

where $T, P, q \geq 0$ are the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$ and, by Theorem 7.2.1, in particular also the threshold, maximum period, and quantifier rank of $\tilde{\varphi}(\overline{x})$.

(Step 2) The algorithm of Theorem 3.2.1 computes, on input of d, σ, and $\tilde{\varphi}(\overline{x})$, a HNF-formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ that is d-equivalent to $\tilde{\varphi}(\overline{x})$ and thus also to $\varphi(\overline{x})$. By Theorem 3.2.1, $\psi(\overline{x})$ has locality radius $\leq 4^q$ and threshold $< T + (n{+}q) \cdot \nu_d(4^q)$, where $n \geq 0$ is the number of free variables of $\varphi(\overline{x})$.

The construction of $\psi(\overline{x})$ from $\tilde{\varphi}(\overline{x})$ takes time in

$$(2\max\{1, T, P\})^{(||\tilde{\varphi}|| \cdot \nu_d(4^q))^{\mathcal{O}(||\sigma||)}}. \tag{2}$$

Combining Estimate (1), which also serves as an upper bound on the size of $\tilde{\varphi}(\overline{x})$, with Estimate (2), we obtain that the algorithm can altogether runs in time

$$\begin{aligned} & (2\max\{1, T, P\})^{\left(\mathcal{O}(||\varphi||) \cdot 2^{\mathcal{O}(q) \cdot (\log \max\{T+1, P\})^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}} \\ \subseteq \quad & 2^{\left(||\varphi|| \cdot 2^{q \cdot (\log \max\{T+1, P\})^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}. \end{aligned}$$

This completes the proof of Theorem 7.3.1. ☐

7.3.2 Nurmonen's Theorem for Tuple-Counting Quantifiers

In the following, we show that the locality theorem for $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$, that is, Theorem 3.3.1, also holds for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$. In particular, no modifications to the preconditions are required. The proof follows directly from the observation that when transforming from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ to $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$, the quantifier rank, the threshold, and the period of the modulo-counting quantifiers in the formulae do not change.

Theorem 7.3.3. *Let σ be a relational signature and let $d \geq 2$ be a degree bound. Furthermore, let $T, n, q \geq 0$, and $M \geq 1$.*

Suppose that $\mathcal{A}$ and $\mathcal{B}$ are d-bounded σ-structures and $\overline{a} \in A^n$, $\overline{b} \in B^n$, such that the following Conditions (1) to (3) are satisfied for $r := 4^q$:

(1) $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \;\cong\; \mathcal{N}_r^{\mathcal{B}}(\overline{b})$.

For every type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$,

(2) $|\tau(\mathcal{A})| \;\equiv\; |\tau(\mathcal{B})| \mod M$, *and*

(3) either $|\tau(\mathcal{A})| \;=\; |\tau(\mathcal{B})|$ *or*

$$|\tau(\mathcal{A})|, |\tau(\mathcal{B})| \;\geq\; T + (n{+}q) \cdot \nu_d(r).$$

Then, for every formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ *with threshold $\leq T$, quantifier rank $\leq q$, at most n free variables $\overline{x}$, and such that M is a common multiple of the periods of all modulo-counting quantifiers that occur in $\varphi(\overline{x})$,*

$$\mathcal{A} \models \varphi[\overline{a}] \quad \textit{iff} \quad \mathcal{B} \models \varphi[\overline{b}].$$

Proof. Let σ be a relational signature and let $d \geq 2$ be a degree bound. Furthermore, let $T, n, q \geq 0$, and $M \geq 1$. Suppose that $\mathcal{A}$ and $\mathcal{B}$ are d-bounded σ-structures and $\overline{a} \in A^n$, $\overline{b} \in B^n$, such that Conditions (1) to (3) of Theorem 7.3.3 are satisfied.

Consider a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ with threshold $\leq T$, quantifier rank $\leq q$, and a tuple $\overline{x}$ of at most n free variables, and such that M is a common multiple of the periods of all modulo-counting quantifiers occurring in $\varphi(\overline{x})$.

By Theorem 7.2.1, $\varphi(\overline{x})$ is equivalent to a formula $\tilde{\varphi}(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$, which also has threshold $\leq T$, quantifier rank $\leq q$, at most n free variables, and where M is also a common multiple of the periods of all modulo-counting quantifiers occurring in the formula. In particular, we know by Theorem 3.3.1 that

$$\mathcal{A} \models \tilde{\varphi}[\overline{a}] \quad \text{iff} \quad \mathcal{B} \models \tilde{\varphi}[\overline{b}].$$

Thus, since $\varphi(\overline{x})$ and $\tilde{\varphi}(\overline{x})$ are equivalent, also

$$\mathcal{A} \models \varphi[\overline{a}] \quad \text{iff} \quad \mathcal{B} \models \varphi[\overline{b}].$$

This completes the proof of Theorem 7.3.3. $\square$

7.3.3 Model-Checking

We conclude the section with a generalisation of the model-checking algorithm for $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ from Theorem 3.4.1 to formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$.

Theorem 7.3.4. *There is an algorithm which, on input of*

- *a formula $\varphi(\overline{x})$ from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$*, where the tuple $\overline{x}$ consists of the $n \geq 0$ free variables of φ,*
- *a finite σ-structure $\mathcal{A}$ (where σ consists of precisely the relation symbols that occur in φ), and a tuple $\overline{a} \in A^n$,*

decides whether $\mathcal{A} \models \varphi[\overline{a}]$.

This algorithm takes time in

$$2^{\left(||\varphi||\cdot 2^{q\cdot(\log\max\{T+1,P\})^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}\cdot||\mathcal{A}||$$

where $T, P, q \geq 0$ are the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$, respectively, and where $d \geq 2$ is a bound on the degree of $\mathcal{A}$.

Remark 7.3.5. Since $T, P, q, ||\sigma|| < ||\varphi||$, the algorithm of Theorem 3.4.1 takes 3-fold exponential time in the size of $\varphi(\overline{x})$ for every σ-structure $\mathcal{A}$ with degree $d \geq 3$, and 2-fold exponential time for every σ-structure $\mathcal{A}$ with degree $d \leq 2$ (and independent of that, linear time in the size of $\mathcal{A}$).

Proof of Theorem 7.3.4. Let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ whose $n \geq 0$ free variables are described by the tuple $\overline{x}$ and where σ consists of precisely the relation symbols that occur in $\varphi(\overline{x})$. Furthermore, let $\mathcal{A}$ be a σ-structure and $\overline{a} \in A^n$.

The algorithm proceeds in the following two steps:

(Step 1) The algorithm of Theorem 7.2.1 constructs for $\varphi(\overline{x})$ an equivalent formula $\tilde{\varphi}(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}[\sigma]$. This takes time in

$$\mathcal{O}(||\varphi||)\cdot 2^{\mathcal{O}(q)\cdot(\log\max\{T+1,P\})^2}, \tag{1}$$

where $T, P, q \geq 0$ are the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$ and, by Theorem 7.2.1, also the threshold, the maximum period, and the quantifier rank of $\tilde{\varphi}(\overline{x})$.

(Step 2) The algorithm of Theorem 3.4.1 decides, on input of $\tilde{\varphi}(\overline{x})$, $\mathcal{A}$, and $\overline{a}$, whether $\mathcal{A} \models \tilde{\varphi}[\overline{a}]$. This takes time in

$$(2\max\{1,T,P\})^{(||\tilde{\varphi}||\cdot\nu_d(4^q))^{\mathcal{O}(||\sigma||)}}\cdot||\mathcal{A}||, \tag{2}$$

where $d \geq 2$ is an upper bound on the degree of $\mathcal{A}$.

Since Estimate (1) is also an upper bound on the size of $\tilde{\varphi}(\overline{x})$, we obtain together with Estimate (2), that to decide whether $\mathcal{A} \models \varphi[\overline{a}]$ takes time in

$$\begin{aligned} & (2\max\{1,T,P\})^{\left(\mathcal{O}(||\varphi||)\cdot 2^{\mathcal{O}(q)\cdot(\log\max\{T+1,P\})^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}\cdot||\mathcal{A}|| \\ \subseteq\ & 2^{\left(||\varphi||\cdot 2^{q\cdot(\log\max\{T+1,P\})^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}\cdot||\mathcal{A}||. \end{aligned}$$

This completes the proof of Theorem 7.3.4. $\square$

7.4 Feferman-Vaught Decompositions

In this section, we apply the transformation of formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ into equivalent formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}$, described in Section 7.2, to Feferman-Vaught decompositions.

The construction of Hanf normal form for $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$, described in the previous section, leads to an algorithm to compute $\oplus$-decompositions for $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ on classes of structures of bounded degree.

Recall that, in Chapter 5, we could construct decompositions with respect to transductions and direct products only for plain FO-formulae. This was due to the tuple-counting quantifiers introduced by computing reducts for suitable transductions. In the present section, we can get rid of this restriction and finally compute such decompositions for arbitrary formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}$ and $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$.

7.4.1 Decompositions with respect to Disjoint Sums

In this section, we generalise the algorithm of Theorem 5.2.1 to formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$. More precisely, we show the following result:

Theorem 7.4.1. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *a relational signature σ,*
- *an arity $s \geq 1$, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}(D)[\sigma_s]$ with $D \subseteq D_{\mathrm{all}}$, $n \coloneqq |\overline{x}|$ free variables, threshold $T \geq 0$, and quantifier rank $q \geq 0$,*

computes an s-ary $\oplus$-decomposition $(\beta, \Delta_1, \ldots, \Delta_s)$ for $\varphi(\overline{x})$ over $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma]$ on $\mathfrak{C}^{d,\sigma}$, where all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF*-formulae with threshold $< T + (n{+}q) \cdot \nu_d(4^q)$.*

Furthermore, the algorithm computes Δ in time

$$2^{\left(||\varphi||\cdot 2^{q\cdot(\log\max\{T+1,P\})^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}}$$

where $P \geq 0$ is the maximum period of $\varphi(\overline{x})$.

Remark 7.4.2. Suppose that σ only contains relation symbols that actually occur in $\varphi(\overline{x})$ and recall that $T, P, q < ||\varphi||$. Then, the algorithm takes 3-fold exponential time

$$2^{d^{s \cdot 2^{\mathcal{O}(||\varphi||)}}}$$

in the size of the input formula for $d = 3$, and, for $d = 2$, 2-fold exponential time

$$2^{2^{s \cdot \mathrm{poly}(||\varphi||)}}.$$

Recall that the algorithm of Theorem 5.2.1 first transformed the input formula into a d-equivalent HNF-formula from $\mathsf{FO{+}unM}$, whose counting-sentences and sphere-formulae subsequently got decomposed separately. For the proof of Theorem 7.4.1, we just have to replace the first step for the construction of HNF-formulae by the corresponding algorithm of Theorem 7.3.1 for formulae from $\mathsf{FO{+}unM}_{\mathrm{tpl}}$.

Proof of Theorem 7.4.1. We describe the algorithm on input of a degree bound $d \geq 2$, a relational signature σ, a number $s \geq 1$, and a formula $\varphi(\overline{x})$ from $\mathsf{FO{+}unM}(D)_{\mathrm{tpl}}[\sigma_s]$ with $D \subseteq D_{\mathrm{all}}$. Let $T, P, q \geq 0$ be the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$, respectively, and let $n := |\overline{x}|$ be the number of free variables of $\varphi(\overline{x})$.

(Step 1) The algorithm of Theorem 7.3.1 constructs, on input of d, σ_s, and $\varphi(\overline{x})$, a HNF-formula $\psi(\overline{x})$ from $\mathsf{FO{+}unM}(D)[\sigma_s]$ that is d-equivalent to $\varphi(\overline{x})$ and that has threshold $< T + (n{+}q) \cdot \nu_d(4^q)$. This takes time in

$$2^{\left(||\varphi|| \cdot 2^{q \cdot (\log \max\{T+1, P\})^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}}. \tag{1}$$

(Step 2) On input of s and $\psi(\overline{x})$, the algorithm of Lemma 5.2.3 computes an s-ary $\oplus$-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ for $\psi(\overline{x})$ over $\mathsf{FO{+}unM}(D)[\sigma]$ on the class of all σ-structures where all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF-formulae with threshold $< T + (n{+}q) \cdot \nu_d(4^q)$.

This takes time in $s \cdot \mathcal{O}(||\psi||)$. Since the size of $\psi(\overline{x})$ is bounded by the time required for its construction, this can also be bounded by Estimate (1).

Clearly, Δ is also an s-ary $\oplus$-decomposition for $\varphi(\overline{x})$ on $\mathfrak{C}^{d,\sigma}$, and the time required by the algorithm to construct Δ can be bounded by Estimate (1). This completes the proof of Theorem 7.4.1.

Note that an alternative proof of Theorem 7.4.1 that uses the algorithms of Theorem 7.2.1 and Theorem 5.2.1 as intermediate steps leads to the same time complexity. $\square$

7.4.2 Decompositions with respect to Transductions

The result of this section enables us to compute decompositions defined by transductions on disjoint sums for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$, thus extending the corresponding results for the special case of FO from Chapter 5. It can be stated as follows:

Theorem 7.4.3. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$,
- *relational signatures* σ *and* τ,
- *an arity* $s \geq 1$,
- *a transduction* Θ *from* σ_s *to* τ *with arity* $t \geq 1$ *and quantifier rank* $q_\Theta \geq 0$, *and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\tau]$ *with* $D \subseteq D_{\mathrm{all}}$, $n := |\overline{x}|$ *free variables, threshold* $T \geq 0$, *and quantifier rank* $q \geq 0$,

computes a Θ*-decomposition* $\Delta = (\beta, \Delta_1, \dots, \Delta_s)$ *over* $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ *for* $\varphi(\overline{x})$ *on* $\mathfrak{C}^{d,\sigma}$, *where all the formulae in the sets* $\Delta_1, \dots, \Delta_s$ *are* HNF*-formulae with threshold* $< T + (t \cdot (n+q) + q_\Theta) \cdot \nu_d(4^{t \cdot q + q_\Theta})$

Furthermore, the algorithm computes Δ *in time*

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + 2^{\left(||\Theta|| \cdot ||\varphi|| \cdot 2^{(t \cdot q + q_\Theta) \cdot (\log \max\{T+1,P\})^2} \cdot \nu_d(4^{t \cdot q + q_\Theta})\right)^{\mathcal{O}(||\sigma_s||)}}$$

and of size

$$2^{\left(||\Theta|| \cdot ||\varphi|| \cdot 2^{(t \cdot q + q_\Theta) \cdot (\log \max\{T+1,P\})^2} \cdot \nu_d(4^{t \cdot q + q_\Theta})\right)^{\mathcal{O}(||\sigma_s||)}}$$

where $P \geq 0$ *is the maximum period of* $\varphi(\overline{x})$.

Remark 7.4.4. Clearly, $T, P, q < ||\varphi||$ and $q_\Theta < ||\Theta||$. Under the assumption that furthermore $||\sigma|| \leq ||\varphi||$ and $t < ||\Theta||$, we can conclude that for every degree bound $d \geq 3$, the algorithm of Theorem 7.4.3 takes time in

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + 2^{d^{s \cdot 2^{||\Theta|| \cdot \mathcal{O}(||\varphi||)}}}.$$

Moreover, for degree bound $d = 2$, the algorithm takes time in

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + 2^{2^{s \cdot ||\Theta|| \cdot \mathrm{poly}(||\varphi||)}}.$$

Proof. Let $d \geq 2$ be a degree bound, let σ and τ be relational signatures, and let $s \geq 1$. Furthermore, let Θ be a transduction from σ_s to τ with arity $t \geq 1$ and quantifier rank $q_\Theta \geq 0$. Moreover, let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma]$ with $D \subseteq D_{\mathrm{all}}$, the $n \geq 0$ free variables $\overline{x} = (x_1, \ldots, x_n)$, threshold $T \geq 0$, and quantifier rank $q \geq 0$. For all $i \in [1, n]$, let $\overline{x}_i = (x_{i,1}, \ldots, x_{i,t})$.

The algorithm proceeds in the two following steps:

(Step 1) The algorithm of Lemma 2.6.4 computes a Θ-reduct $\varphi^{-\Theta}(\overline{x}_1, \ldots, \overline{x}_t)$ for $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma_s]$ that has quantifier rank $\leq t \cdot q + q_\Theta$, $n \cdot t$ free variables, and the same threshold and maximum period as $\varphi(\overline{x})$. This takes time in

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + ||\Theta|| \cdot \mathcal{O}(||\varphi||),$$

and $\Theta^{-1}(\varphi)(\overline{x}_1, \ldots, \overline{x}_t)$ has size in $||\Theta|| \cdot \mathcal{O}(||\varphi||)$.

(Step 2) The algorithm of Theorem 7.4.1 computes, on input of d, σ, s, and $\varphi^{-\Theta}(\overline{x}_1, \ldots, \overline{x}_t)$, an s-ary $\oplus$-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ for $\varphi^{-\Theta}(\overline{x}_1, \ldots, \overline{x}_t)$ over $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ on $\mathfrak{C}^{d,\sigma}$, where the sets $\Delta_1, \ldots, \Delta_s$ only contain HNF-formulae with threshold less than $T + (t \cdot (n + q) + q_\Theta) \cdot \nu_d(4^{t \cdot q + q_\Theta})$. This takes time in

$$2^{\left(||\Theta|| \cdot ||\varphi|| \cdot 2^{(t \cdot q + q_\Theta) \cdot (\log \max\{T+1, P\})^2} \cdot \nu_d(4^{t \cdot q + q_\Theta})\right)^{\mathcal{O}(||\sigma_s||)}},$$

where $P \geq 0$ is the maximum period of $\varphi(\overline{x})$. Note that the latter estimate also bounds the size of Δ.

By Lemma 5.3.2, we know that Δ is also a Θ-decomposition for $\varphi(\overline{x})$ over $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ on the class of d-bounded σ-structures.

Altogether, the algorithm takes time in

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + 2^{\left(||\Theta|| \cdot ||\varphi|| \cdot 2^{(t \cdot q + q_\Theta) \cdot (\log \max\{T+1, P\})^2} \cdot \nu_d(4^{t \cdot q + q_\Theta})\right)^{\mathcal{O}(||\sigma_s||)}}$$

to compute Δ. This completes the proof of Theorem 7.4.3. $\square$

7.4.3 Decompositions with respect to Direct Products

We conclude Section 7.4 by an application of Theorem 7.4.3, which provides us with an algorithm to compute $\otimes$-decompositions for $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ on classes of structures of bounded degree. More precisely, we show the following:

Theorem 7.4.5. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *a relational signature σ,*
- *an arity $s \geq 1$, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma_s]$ with $D \subseteq D_{\mathrm{all}}$, $n := |\overline{x}|$ free variables, threshold $T \geq 0$, and quantifier rank $q \geq 0$,*

computes an s-ary $\otimes$-decomposition $(\beta, \Delta_1, \ldots, \Delta_s)$ for $\varphi(\overline{x})$ over $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ on $\mathfrak{C}^{d,\sigma}$, where all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF*-formulae with threshold $< T + s \cdot (n{+}q) \cdot \nu_d(4^{s \cdot q})$.*

Furthermore, the algorithm computes Δ in time

$$2^{\left(||\varphi|| \cdot 2^{q \cdot (\log \max\{T+1, P\})^2} \cdot \nu_d(4^{s \cdot q})\right)^{\mathcal{O}(||\sigma_s|| \cdot \log ||\sigma_s||)}}$$

where $P \geq 0$ is the maximum period of φ.

Remark 7.4.6. Clearly, $T, P, q < ||\varphi||$. Under the assumption that furthermore $||\sigma|| < ||\varphi||$, we can conclude that for every degree bound $d \geq 3$, the algorithm of Theorem 7.4.5 takes time in

$$2^{d^{2^{s \cdot \mathcal{O}(||\varphi||)}}}.$$

Moreover, for degree bound $d = 2$, the algorithm takes time in

$$2^{2^{s \cdot \mathrm{poly}(||\varphi||)}}.$$

Proof. Let $d \geq 2$, let σ be a relational signature, and let $s \geq 1$. Furthermore, let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}[\sigma_s]$ with $D \subseteq D_{\mathrm{all}}$, threshold $T \geq 0$, and quantifier rank $q \geq 0$.

On input of d, the signatures σ_s and σ, the transduction Θ_s^{δ}, defined in Section 5.4, and the formula $\varphi(\overline{x})$, the algorithm of Theorem 7.4.3 computes a Θ_s^{σ}-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ over $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ for $\varphi(\overline{x})$ on $\mathfrak{C}^{d,\sigma}$

where all formulae in the sets $\Delta_1, \dots, \Delta_s$ are HNF-formulae with threshold $< T + s \cdot (n+q) \cdot \nu_d(4^{s \cdot q})$.

By Lemma 5.4.2, we know that Δ is also $\otimes$-decomposition for $\varphi(\overline{x})$ over $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ on $\mathfrak{C}^{d,\sigma}$.

Time complexity. The transduction Θ_s^σ is of quantifier rank 0 and can be computed in time $s \cdot \mathcal{O}(||\sigma||)$. Therefore, the call of the algorithm of Theorem 7.4.3 needs time in

$$\begin{aligned} & s \cdot \mathcal{O}(||\sigma||)^2 + 2^{\left(s \cdot ||\sigma|| \cdot ||\varphi|| \cdot 2^{s \cdot q \cdot (\log \max\{T+1,P\})^2} \cdot \nu_d(4^{s \cdot q})\right)^{\mathcal{O}(||\sigma_s||)}} \\ \subseteq \quad & 2^{\left(||\varphi|| \cdot 2^{q \cdot (\log \max\{T+1,P\})^2} \cdot \nu_d(4^{s \cdot q})\right)^{\mathcal{O}(||\sigma_s|| \cdot \log ||\sigma_s||)}}, \end{aligned}$$

where $P \geq 0$ is the maximum period of φ. This completes the proof of Theorem 7.4.5. $\square$

7.5 Preservation Theorems

In Chapter 6, we have shown how formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ that are preserved under extensions (homomorphisms) on a class of structures of bounded degree that is closed under disjoint unions and induced substructures (and, for preservation under homomorphisms, decidable in 1-fold exponential time) can be turned into existential (existential-positive) formulae in elementary time.

In this section, we generalise these results from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ to $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$.

7.5.1 Preservation under Extensions

In this section, we show the following generalisation of Theorem 6.1.7:

Theorem 7.5.1. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *a relational signature σ, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$,*

constructs an existential formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ such that the following holds for any class $\mathfrak{D}$ of d-bounded σ-structures that is closed under disjoint unions and induced substructures: If $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{D}$, then $\varphi(\overline{x})$ and $\psi(\overline{x})$ are $\mathfrak{D}$-equivalent.

Furthermore, the algorithm computes $\psi(\overline{x})$ in time

$$||\varphi|| \cdot \left(2^{\nu_d(2^{\nu_d(4^q)^{\mathcal{O}(||\sigma||)}})} \cdot (T{+}n{+}q) \cdot L\right)^{(n+q)\cdot\mathcal{O}((\log\max\{1,T,P\})^2)},$$

where $T, P, n, q \geq 0$ and $L \geq 1$ are the threshold, the maximum period, the number of free variables, the quantifier rank, and the least common multiple of the periods of all modulo-counting quantifiers in $\varphi(\overline{x})$, respectively. In particular, the constants suppressed by the $\mathcal{O}$-notation do not depend on the signature σ.

Remark 7.5.2. In particular, if we assume that σ only contains relation symbols that actually occur in $\varphi(\overline{x})$, then the algorithm of Theorem 7.5.1 takes 5-fold exponential time in the size of $\varphi(\overline{x})$ for degree bounds $d \geq 3$, and 3-fold exponential time for $d = 2$.

The main tasks of the proof of Theorem 7.5.1 are, analogous to the proof of Theorem 6.1.7, an upper bound on the size of minimal models for the input formula, and the construction of an existential formula using this upper bound. We first focus on these tasks and prove Theorem 7.5.1 afterwards.

For the first task, it turns out that the upper bound on the size of minimal models, stated in Theorem 6.2.1 for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$, also holds for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$. This is due to the fact that, by Theorem 7.2.1, each formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ is equivalent to a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ over the same signature, with the same threshold and quantifier rank, and with modulo-counting quantifiers of the same periods. Another way to see this is to just replace the use of Theorem 3.3.1 in the proof of Theorem 6.2.1 by Theorem 7.3.3.

In the following corresponding corollary to Theorem 6.2.1, we use the expression $S^{d,s}(r) := 2^{\nu_d(r)^{\mathcal{O}(s)}}$ as introduced in Chapter 6.

Corollary 7.5.3. *There is a function*

$$N^{d,||\sigma||}(T,n,q,L) \quad \in \quad S^{d,||\sigma||}(S^{d,||\sigma||}(4^q)) \cdot (T{+}n{+}q) \cdot L,$$

such that the following holds for every relational signature σ, every degree bound $d \geq 2$, every class $\mathfrak{D}$ of d-bounded σ-structures that is closed under disjoint unions and induced substructures, and every formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$:

If $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{D}$, then every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of size at most $N^{d,||\sigma||}(T,n,q,L)$, where $T, n, q \geq 0$ are the threshold, the number of free variables, and the quantifier rank of $\varphi(\overline{x})$, and where $L \geq 1$ is the least common multiple of the periods of all modulo-counting quantifiers that appear in $\varphi(\overline{x})$.

Proof. Let σ be a relational signature, let $d \geq 2$, and let $\mathfrak{D}$ be a class of d-bounded σ-structures that is closed under disjoint unions and induced substructures.

Furthermore, let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ that is preserved under extensions on $\mathfrak{D}$. Let $D \subseteq D_{\mathrm{all}}$ be the set of all modulo-counting quantifiers that occur in φ, let $T, q \geq 0$ be the threshold and the quantifier rank of φ, let $n := |\overline{x}|$ be the number of free variables of $\varphi(\overline{x})$, and let $L \geq 1$ be the least common multiple of the periods of all modulo-counting quantifiers in the set D.

By Theorem 7.2.1, there is a formula $\tilde{\varphi}(\overline{x})$, equivalent to $\varphi(\overline{x})$, in $\mathsf{FO}+\mathrm{un}\mathsf{M}(D)[\sigma]$ that has the same threshold T, the same quantifier rank q, and the same number of free variables as $\varphi(\overline{x})$, and where L is also the least common multiple of the periods of all modulo-counting quantifiers appearing in $\tilde{\varphi}(\overline{x})$.

Let $N := N^{d,||\sigma||}(T, n, q, L)$ be the upper bound on the size of $\mathfrak{D}$-minimal models of $\tilde{\varphi}(\overline{x})$, provided by Theorem 6.2.1. Since $\varphi(\overline{x})$ and $\tilde{\varphi}(\overline{x})$ are equivalent, N is also an upper bound on the size of the $\mathfrak{D}$-minimal models of $\varphi(\overline{x})$.

This completes the proof of Corollary 7.5.3. $\square$

The following corollary extends Lemma 6.2.2 from $\mathsf{FO}+\mathrm{un}\mathsf{M}$ to $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$.

Corollary 7.5.4. *There is an algorithm which, on input of*

- *a number $N \geq 1$ and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ over a relational signature σ whose $n \geq 0$ free variables are the variables of the tuple $\overline{x}$,*

constructs an existential formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ such that the following holds for every class $\mathfrak{C}$ of σ-structures that is closed under induced substructures:

If $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{C}$ and every $\mathfrak{C}$-minimal model of $\varphi(\overline{x})$ has a universe of size $\leq N$, then $\psi(\overline{x})$ is $\mathfrak{C}$-equivalent to $\varphi(\overline{x})$.

Furthermore, the algorithm constructs $\psi(\overline{x})$ in time

$$\mathcal{O}(||\varphi||) \cdot 2^{(n+q)\cdot(\log \max\{T+1,P\})^2 \cdot \mathcal{O}(\log N)},$$

where $T, P, q \geq 0$ are the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$, respectively. The constant suppressed by the $\mathcal{O}$-notation does not depend on the signature σ.

Proof. Let σ be a relational signature, let $N \geq 1$, and let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ with $n := |\overline{x}|$ free variables. Let $D \subseteq D_{\mathrm{all}}$ be the set of all modulo-counting quantifiers in $\varphi(\overline{x})$, and let $T, P, q \geq 0$ be the threshold, the maximum period, and the quantifier rank of $\varphi(\overline{x})$, respectively.

(Step 1) By Theorem 7.2.1, a formula $\tilde{\varphi}(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)[\sigma]$ that is equivalent to $\varphi(\overline{x})$ and that has the same threshold and quantifier rank as $\varphi(\overline{x})$ can be computed in time

$$\mathcal{O}(||\varphi||) \cdot 2^{\mathcal{O}(q)\cdot(\log\max\{T+1,P\})^2}. \tag{1}$$

and of size bounded by the same expression.

(Step 2) The algorithm of Lemma 6.2.2 computes, on input of N and $\tilde{\varphi}(\overline{x})$, an existential formula $\varphi_N(\overline{x})$ from $\mathsf{FO}[\sigma]$ such that the following holds for every class $\mathfrak{C}$ of σ-structures that is closed under induced substructures:

If $\tilde{\varphi}(\overline{x})$ (and thus, $\varphi(\overline{x})$) is preserved under extensions on $\mathfrak{C}$ and every $\mathfrak{C}$-minimal model of $\tilde{\varphi}(\overline{x})$ (and thus, of $\varphi(\overline{x})$) has a universe of size $\leq N$, then $\varphi_N(\overline{x})$ is $\mathfrak{C}$-equivalent to $\tilde{\varphi}(\overline{x})$ and $\varphi(\overline{x})$.

This takes time in

$$||\tilde{\varphi}|| \cdot (2\max\{1,T,P\})^{(n+q)\cdot\mathcal{O}(\log N)}. \tag{2}$$

Putting Estimate (1) and Estimate (2) together, we obtain that the construction of $\varphi_N(\overline{x})$ altogether takes time in

$$\mathcal{O}(||\varphi||) \cdot 2^{(n+q)\cdot(\log\max\{T+1,P\})^2\cdot\mathcal{O}(\log N)}.$$

This completes the proof of Corollary 7.5.4. □

We are now ready to prove Theorem 7.5.1 by using Corollary 7.5.3 and Corollary 7.5.4. The proof has the same overall shape as the proof of Theorem 6.1.7.

Proof of Theorem 7.5.1. Let $d \geq 2$ be a degree bound, let σ be a relational signature, and let $\varphi(\overline{x})$ be an $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$-formula with $n := |\overline{x}|$ free variables, threshold $T \geq 0$, maximum period $P \geq 0$, and quantifier rank $q \geq 0$. Furthermore, let $L \geq 1$ be the least common multiple of the periods of all modulo-counting quantifiers occurring in $\varphi(\overline{x})$.

Let $\mathfrak{D}$ be a class of d-bounded σ-structures that is closed under disjoint unions and induced substructures and suppose that $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{D}$.

The algorithm proceeds in the following two steps:

(Step 1) Compute the upper bound

$$\begin{aligned} N &:= N^{d,||\sigma||}(T,n,q,L) \\ &\in S^{d,||\sigma||}(S^{d,||\sigma||}(4^q)) \cdot (T{+}n{+}q) \cdot L \end{aligned} \tag{1}$$

on the size of $\mathfrak{D}$-minimal models of $\varphi(\overline{x})$, obtained from Corollary 7.5.3. In particular, we can assume that $N \geq 2$.

(Step 2) The algorithm of Corollary 7.5.4 constructs an existential formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ that is $\mathfrak{D}$-equivalent to $\varphi(\overline{x})$. This takes time in

$$\begin{aligned} & \mathcal{O}(||\varphi||) \cdot 2^{(n+q)\cdot(\log\max\{T+1,P\})^2\cdot\mathcal{O}(\log N)} \\ \subseteq \quad & ||\varphi|| \cdot N^{(n+q)\cdot\mathcal{O}((\log\max\{1,T,P\})^2)}. \end{aligned}$$

Thus, by replacing N in the latter estimate with Estimate (1) and recalling the definition of $S^{\cdot,\cdot}(\cdot)$, we obtain that $\psi(\overline{x})$ can altogether be computed in time

$$||\varphi|| \cdot \Big(2^{\nu_d(2^{\nu_d(4^q)^{\mathcal{O}(||\sigma||)}})} \cdot (T{+}n{+}q) \cdot L\Big)^{(n+q)\cdot\mathcal{O}((\log\max\{1,T,P\})^2)}.$$

This completes the proof of Theorem 6.1.7. $\square$

7.5.2 Preservation under Homomorphisms

In this section, we show the following generalisation of Theorem 6.1.10:

Theorem 7.5.5. *Let $\mathfrak{C}'$ a class of structures that is decidable in time $t(n)$ for some function $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$ and that is closed under disjoint unions and induced substructures.*

There is an algorithm which, on input of

- *a degree bound $d \geq 2$,*
- *a relational signature σ, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{unM}_{\mathrm{tpl}}[\sigma]$,*

constructs an existential-positive formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ such that the following holds for the class $\mathfrak{D}$ of d-bounded σ-structures from $\mathfrak{C}'$: If $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, then $\varphi(\overline{x})$ and $\psi(\overline{x})$ are $\mathfrak{D}$-equivalent.

Furthermore, the algorithm computes $\psi(\overline{x})$ in time

$$2^{||\varphi||\cdot(n+1)^{\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}} \cdot t\big((n+1)^{\mathcal{O}(||\sigma||)} \cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}\big),$$

where $n, q \geq 0$ are the number of free variables and the quantifier rank of $\varphi(\overline{x})$, respectively; and the formula $\psi(\overline{x})$ is of size

$$2^{(n+1)^{\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}}.$$

Remark 7.5.6. In particular, if $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$ is at most 1-fold exponential and if we assume that σ only contains relation symbols that actually occur in the input formula φ, then the algorithm of Theorem 7.5.5 takes 4-fold exponential time in the size of $\varphi(\overline{x})$ for degree bounds $d \geq 3$, and 3-fold exponential time for $d = 2$.

The proof of Theorem 7.5.5 has the same structure as the one of Theorem 6.1.10. In the first step, we find upper bounds on the size of the minimal models of formulae from $\mathsf{FO}{+}\mathrm{unM}_{\mathrm{tpl}}$. It turns out that these upper bounds are precisely the same as the ones for formulae from $\mathsf{FO}{+}\mathrm{unM}$ stated in Theorem 6.3.1. In the second step, we use Lemma 6.3.2 again to construct existential-positive formulae using this upper bound.

Corollary 7.5.7. *There is a function*

$$N^{d,||\sigma||}(n,q) \quad \in \quad (n{+}1) \cdot S^{d,||\sigma||}(2 \cdot 4^q)$$

such that the following holds for every relational signature σ, every degree bound $d \geq 2$, every class $\mathfrak{D}$ of d-bounded σ-structures that is closed under disjoint unions and induced substructures, and every formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{unM}_{\mathrm{tpl}}[\sigma]$:

If $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, then every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of size at most $N^{d,||\sigma||}(n,q)$, where $n, q \geq 0$ are the number of free variables and the quantifier rank of φ, respectively.

Proof. Let σ be a relational signature, let $d \geq 2$ be a degree bound, and let $\mathfrak{D}$ be a class of d-bounded σ-structures that is closed under disjoint unions and induced substructures.

Let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{unM}_{\mathrm{tpl}}[\sigma]$ with $n \geq 0$ free variables and quantifier rank $q \geq 0$. By Theorem 7.2.1 there is a formula $\tilde{\varphi}(\overline{x})$ in $\mathsf{FO}{+}\mathrm{unM}[\sigma]$ with the same number of free variables and the same quantifier rank as $\varphi(\overline{x})$ and that is equivalent to $\varphi(\overline{x})$.

Suppose that $\varphi(\overline{x})$ and $\tilde{\varphi}(\overline{x})$ are preserved under homomorphisms on $\mathfrak{D}$. By Theorem 6.3.1, every $\mathfrak{D}$-minimal model of $\tilde{\varphi}(\overline{x})$ has a universe of size at most $N^{d,||\sigma||}(n,q)$ for the function provided by Theorem 6.3.1. Since $\varphi(\overline{x})$ and $\tilde{\varphi}(\overline{x})$ are equivalent, the same holds also for $\varphi(\overline{x})$. Thus, the proof of Corollary 7.5.7 is completed, since we can choose the same function as in Theorem 6.3.1 for an upper bound on the size of minimal models. $\square$

With this, we are ready to prove Theorem 7.5.5.

Proof sketch of Theorem 7.5.5. The proof of Theorem 7.5.5 proceeds in exactly the same fashion and with the same estimates as the proof of Theorem 6.1.10.

The only difference is the use of Corollary 7.5.7 instead of Theorem 6.3.1 for the upper bound on the size of minimal models. □

7.6 Conclusion

In this chapter, we have extended our results from the previous chapters to the logic $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$, that is, the extension of first-order logic by threshold- and modulo-counting quantifiers over tuples.

To this aim, we have used a construction (described in, e.g., [Str94]) that turns formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ into equivalent formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}$. This transformation takes linear time in the size of the input formula and exponential time in its quantifier rank, and yields formulae with the same threshold and with the same modulo-counting quantifiers.

Using this construction, the extensions of our algorithmic results from Chapter 3, Chapter 5, and Chapter 6 have roughly the same running time as for the special case of $\mathsf{FO}+\mathrm{un}\mathsf{M}$.

For the following summary, we focus on degree bounds $d \geq 3$. In particular, we have shown that formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ can be turned into d-equivalent HNF-formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}$ in 3-fold exponential time. Using these HNF-formulae, we can perform model-checking for formulae φ from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ and structures $\mathcal{A}$ of degree at most d in 3-fold exponential time in the size of φ and linear time in the size of $\mathcal{A}$. Furthermore, the existence of HNF-formulae for $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ leads to a locality theorem in the manner of Nurmonen's theorem for $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$.

Concerning Feferman-Vaught decompositions, we have shown that formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ can, on classes of structures of bounded degree, be decomposed in respect to disjoint sums, transductions on disjoint sums, and in particular, direct products. Each of the corresponding algorithms takes 3-fold exponential time. For decompositions with respect to disjoint sums, this just generalised our result for $\mathsf{FO}+\mathrm{un}\mathsf{M}$ from Section 5.2 to $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$. On the other hand, only the transformation from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ to $\mathsf{FO}+\mathrm{un}\mathsf{M}$, obtained in the present chapter, allowed us to also efficiently construct decompositions for $\mathsf{FO}+\mathrm{un}\mathsf{M}$ with respect to transductions of arity ≥ 2 and, in particular, direct products.

Finally, our algorithmic versions of preservation theorems, described in Chapter 6, could be extended from input formulae of $\mathsf{FO}+\mathrm{un}\mathsf{M}$ to input formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$.

After generalising from quantifiers that count single elements to tuple-counting quantifiers in this chapter, the next chapter aims to extend our results from modulo-counting quantifiers to other unary counting quantifiers.

8 Ultimately Periodic Quantifiers

In this chapter, we show that all results of the previous chapters (apart from Gaifman normal form) can be generalised to extensions of first-order logic by so-called *ultimately periodic* counting quantifiers. We will also show that ultimately periodic counting quantifiers are actually the largest class of unary counting quantifiers for which, in particular, Hanf normal form and Feferman-Vaught style decompositions with respect to disjoint sums are possible at all. This chapter is based on [HKS16].

8.1 Introduction

The main technical difficulties in the constructions described in the earlier chapters of this thesis already lie in the handling of formulae with only threshold-counting and modulo-counting quantifiers. There, we implicitly used that sets C of threshold-counting and modulo-counting quantifiers are *additive*. Intuitively, this means that statements about the sum $n+m$ of two summands n and m using a quantifier from C can be expressed by statements about the individual summands n and m that also only use the quantifiers from C. More precisely, statements of the shape "$n + m \in (\mathsf{Q}{+}k)$" for quantifiers $\mathsf{Q} \in C$ can be expressed by Boolean combinations of statements of the shape "$n \in (\mathsf{R}{+}\ell)$" and "$m \in (\mathsf{R}{+}\ell)$" using quantifiers R which are either from the set C or the existential quantifier. In this chapter, we show that our results actually hold for all additive sets of unary counting quantifiers.

Ultimately periodic quantifiers (cf., e.g., [Mat94]) were introduced in Section 2.5. We will see that sets of unary counting quantifiers are additive if and only if all its quantifiers are ultimately periodic. In particular, the transformations involved in showing that sets of ultimately periodic counting quantifiers are additive will allow us to generalise the results of Chapter 3, Chapter 5, Chapter 6, and Chapter 7 to all ultimately periodic logics. The transformation as well as the resulting construction of Hanf normal form for ultimately periodic logics and a corresponding generalisation of Seese's model-checking algorithm [See96] were already published in [HKS16].

On the other hand, our argument to show that *only* sets of ultimately periodic counting quantifiers are additive will be used to show that ultimately periodic logics are also the only logics that permit Hanf normal form and decompositions with respect to disjoint sums. This is based on a proof in [HKS16].

For a precise definition of additivity, we let P be a unary relation symbol.

Definition 8.1.1. A set $C \subseteq C_{\text{all}}$ is *additive* if for each $\mathsf{Q} \in C \cup \{\exists\}$ and all $k \geq 0$, there is a Boolean combination[1] $\delta^{(\mathsf{Q}+k)}$ of $\mathsf{FO}+\text{un}\mathsf{C}(C)[P]$-sentences of the shape

$$(\mathsf{R}+\ell)y\,P(y) \qquad \text{or} \qquad (\mathsf{R}+\ell)y\,\neg P(y),$$

with $\mathsf{R} \in C \cup \{\exists\}$ and $\ell \geq 0$, such that for every (P)-structure $\mathcal{A}$,

$$|A| \ \in \ (\mathsf{Q}+k) \quad \text{iff} \quad \mathcal{A} \ \models \ \delta^{(\mathsf{Q}+k)}.$$

Example 8.1.2. The following observations were already used in Section 2.9.

Every set $D \subseteq D_{\text{all}}$ is additive: For each modulo-counting quantifier $\mathsf{D}_p \in D$ and for every $k \geq 0$, the Boolean combination $\delta^{(\mathsf{Q}+k)}$ can be chosen as the disjunction over all formulae

$$(\mathsf{D}_p+\ell_1)y\,P(y) \ \wedge \ (\mathsf{D}_p+\ell_2)y\,\neg P(y)$$

where $0 \leq \ell_1, \ell_2 \leq \max\{k, p\}$ such that $\ell_1 + \ell_2 \geq k$ and $\ell_1 + \ell_2 \equiv k \mod p$.

Moreover, for each $k \geq 0$, $\delta^{(\exists+k)}$ can be chosen as the disjunction of the formulae $\exists^{>k}y\,P(y)$ and $\exists^{>k}y\,\neg P(y)$, as well as all formulae

$$\exists^{>\ell_1}y\,P(y) \ \wedge \ \exists^{>\ell_2}y\,\neg P(y)$$

where $\ell_1, \ell_2 \in [0, k)$ and $(\ell_1{+}1) + (\ell_2{+}1) = k{+}1$.

In Section 8.2, we will prove that only sets of ultimately periodic quantifiers are additive (see Lemma 8.2.1). For the other direction of the characterisation, Lemma 8.3.1 in Section 8.3 transforms formulae from a logic $\mathsf{FO}+\text{un}\mathsf{C}(U)_{\text{tpl}}$ with $U \subseteq U_{\text{all}}$ into equivalent formulae from the logic $\mathsf{FO}+\text{un}\mathsf{M}_{\text{tpl}}$ over the same signature and with the same dimension, which only use modulo-counting quantifiers from the set

$$D^U \ := \quad \{\mathsf{D}_p \,:\, U \text{ contains a quantifier with period } p \geq 2\}.$$

[1] Recall that we only consider *finite* Boolean combinations

Section 8.3 also provides the means to transform formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}(D^U)_{\mathrm{tpl}}$ back into equivalent formulae from $\mathsf{FO}+\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}$ (see Lemma 8.3.5).

Together with Example 8.1.2, this already shows the following observation:

Observation 8.1.3. *The following characterisation holds for any set $C \subseteq C_{\mathrm{all}}$:*

C is additive iff C only contains ultimately periodic quantifiers.

Since the transformations between formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}(U)_{\mathrm{tpl}}$ and formulae from $\mathsf{FO}+\mathrm{un}\mathsf{M}(D^U)_{\mathrm{tpl}}$, described in Section 8.3, are algorithmic, we can use them in the subsequent sections of this chapter to extend our algorithm for the construction of Hanf normal form (see Section 8.4) to ultimately periodic logics. This result was already published in [HKS16].

In the same way, we can generalise the algorithms for Feferman-Vaught style decompositions (see Section 8.5) and existential (existential-positive) formulae for formulae that are preserved under extensions (homomorphisms) on classes of structures of bounded degree (see Section 8.6) to formulae with ultimately periodic quantifiers.

For formulae φ from ultimately periodic logics, we introduce a parameter which, in a sense, generalises the threshold and the maximum period of $\mathsf{FO}+\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$-formulae. The *quantifier weight* is the maximum of 2 and the size $||\mathsf{Q}||$ of all quantifiers Q that occur in φ. Note that the quantifier weight is defined to be at least 2 in order to avoid special cases for quantifier-free formulae in the estimates made in the sequel.

8.2 Only Ultimately Periodic Quantifiers are Additive

In this section, we show that only sets of ultimately periodic quantifiers are additive. Actually, we prove the following stronger result, saying that, for a non-ultimately periodic counting quantifier S, the statement "$|A| \in \mathsf{S}$" for structures $\mathcal{A}$ with a single unary relation $P^{\mathcal{A}}$ cannot be expressed by an equivalent Boolean combination of sentences of the shape $\mathsf{Q}y\,P(y)$ and $\mathsf{Q}y\,\neg P(y)$ for *arbitrary* unary counting quantifiers $\mathsf{Q} \in C_{\mathrm{all}}$.

In Section 8.4 and Section 8.5, we will use Lemma 8.2.1 below to show that logics that allow quantifiers that are not ultimately periodic neither permit Hanf normal form nor Feferman-Vaught decompositions with respect to disjoint sums.

Lemma 8.2.1. *Let P be a unary relation symbol, and let $\mathsf{S} \subseteq \mathbb{N}$ be a unary counting quantifier that is not ultimately periodic.*

Then, there is no Boolean combination ψ of sentences of the shape

$$\mathsf{Q}y\, P(y) \quad \textit{and} \quad \mathsf{Q}y\, \neg P(y)$$

with $\mathsf{Q} \in C_{\mathrm{all}}$, such that

$$\mathcal{A} \models \psi \quad \textit{iff} \quad |A| \in \mathsf{S}$$

for all (P)-structures $\mathcal{A}$.

Proof. Let $\mathsf{S} \subseteq \mathbb{N}$ be a unary counting quantifier that is not ultimately periodic. Let ψ be a Boolean combination of sentences of the shape

$$\mathsf{Q}y\, P(y) \quad \text{and} \quad \mathsf{Q}y\, \neg P(y) \tag{1}$$

with $\mathsf{Q} \in C_{\mathrm{all}}$. We will show that ψ does not expresses "$|A| \in \mathsf{S}$".

Since ψ is finite, there is a finite set $C_\psi \subset C_{\mathrm{all}}$ such that $\mathsf{Q} \in C_\psi$ in each of the sentences of Shape (1) that ψ is built of.

Let $n \in \mathbb{N}_{\geq 1}$ and let $\mathsf{Q}_1, \mathsf{Q}_2, \ldots, \mathsf{Q}_n$ be an enumeration of all $\mathsf{Q} \in C_\psi$. For each $j \in \mathbb{N}$ consider the bit string w_j of length n, defined as

$$w_j \;:=\; w_{1,j} w_{2,j} \;\cdots\; w_{n,j},$$

where, for each $i \in [1, n]$,

$$w_{i,j} \;:=\; \begin{cases} 1 & \text{if } j \in \mathsf{Q}_i, \text{ and} \\ 0 & \text{if } j \notin \mathsf{Q}_i. \end{cases}$$

Since there is only a finite number of bit strings of length n, the following claim holds:

Claim 1. *There are natural numbers $b > a \geq 1$ such that $w_a = w_b$, that is, for all $i \in [1, n]$,*

$$a \in \mathsf{Q}_i \quad \textit{iff} \quad b \in \mathsf{Q}_i.$$

If, for all $c \in \mathbb{N}$, we have $a + c \in \mathsf{S}$ if and only if $b + c \in \mathsf{S}$, then S is ultimately periodic (with period dividing $b - a$ and offset a). Since this is not the case, the following claim holds:

Claim 2. *There is a number $c \in \mathbb{N}$ such that*

$$a + c \;\in\; \mathsf{S} \quad \textit{iff} \quad b + c \;\notin\; \mathsf{S}.$$

Now consider (P)-structures $\mathcal{A}$ and $\mathcal{B}$ with $|A| = a + c$, $|B| = b + c$, and $|P^{\mathcal{A}}| = |P^{\mathcal{B}}| = c$. By Claim 2, we have

$$|A| \in \mathsf{S} \quad \text{iff} \quad |B| \notin \mathsf{S}. \tag{2}$$

Nevertheless, we can show that $\mathcal{A}$ and $\mathcal{B}$ cannot be distinguished by any of the sentences of Shape (1) that occur in ψ. To this end, consider a quantifier $\mathsf{Q}_i \in C_\psi$ for an $i \in [1, n]$.

(Case 1) For the sentence $\mathsf{Q}_i y\, P(y)$, we have

$$\begin{array}{lrcll} & \mathcal{A} & \models & \mathsf{Q}_i y\, P(y) & \\ \text{iff} & |P^{\mathcal{A}}| & \in & \mathsf{Q}_i & \\ \text{iff} & |P^{\mathcal{B}}| & \in & \mathsf{Q}_i & (\text{since } |P^{\mathcal{A}}| = |P^{\mathcal{B}}|) \\ \text{iff} & \mathcal{B} & \models & \mathsf{Q}_i y\, P(y). & \end{array}$$

(Case 2) For the sentence $\mathsf{Q}_i y\, \neg P(y)$, we have

$$\begin{array}{lrcll} & \mathcal{A} & \models & \mathsf{Q}_i y\, \neg P(y) & \\ \text{iff} & |A \setminus P^{\mathcal{A}}| & \in & \mathsf{Q}_i & \\ \text{iff} & a & \in & \mathsf{Q}_i & (\text{since } |A \setminus P^{\mathcal{A}}| = a) \\ \text{iff} & b & \in & \mathsf{Q}_i & (\text{by Claim 1}) \\ \text{iff} & |B \setminus P^{\mathcal{B}}| & \in & \mathsf{Q}_i & (\text{since } |B \setminus P^{\mathcal{B}}| = b) \\ \text{iff} & \mathcal{B} & \models & \mathsf{Q}_i y\, \neg P(y). & \end{array}$$

In summary, the structures $\mathcal{A}$ and $\mathcal{B}$ satisfy the same counting-sentences that occur in ψ. As ψ is a Boolean combination of these counting-sentences, we obtain that

$$\mathcal{A} \models \psi \quad \text{iff} \quad \mathcal{B} \models \psi.$$

Thus, it follows from Equivalence (2) that ψ does not expresses "$|A| \in \mathsf{S}$". $\square$

We can conclude that any set $C \subseteq C_{\text{all}}$ that contains a quantifier S that is not ultimately periodic is not additive, as the Boolean combination δ^{S} from Definition 8.1.1 would be a contradiction to Lemma 8.2.1.

8.3 Modulo-Counting versus Ultimately-Periodic Quantifiers

Let $U \subseteq U_{\text{all}}$ be a set of ultimately periodic quantifiers. In this section, we show how formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\text{tpl}}$ can be turned into equivalent formulas from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\text{tpl}}$ (see Section 8.3.1), and, for a special case, the other way round (see Section 8.3.2).

Note that, although we state the result of Section 8.3.1 for formulae with dimension ≥ 1, this does not add any difficulty to the corresponding proofs, that is, the proofs are identical to the ones for the restriction to dimension 1.

8.3.1 From Ultimately Periodic to Modulo-Counting Quantifiers

This section shows how a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\text{tpl}}$ can be turned into an equivalent formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\text{tpl}}$ with the same dimension and quantifier rank. The following Lemma 8.3.1 is the main result of this section and describes this transformation.

Lemma 8.3.1. *There is an algorithm which, on input of a formula φ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\text{tpl}}$, for a set $U \subseteq U_{\text{all}}$, computes an equivalent formula $\tilde{\varphi}$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\text{tpl}}$.*

The constructed formula $\tilde{\varphi}$ has the same signature, the same quantifier rank, the same free variables, and the same dimension as φ, and it has threshold $< w$, where $w \geq 2$ is the quantifier weight of φ.

Furthermore, the algorithm constructs $\tilde{\varphi}$ from φ in time

$$\mathcal{O}(||\varphi||) \cdot \mathcal{O}(w)^q,$$

where $q \geq 0$ is the quantifier rank of φ.

The proof of Lemma 8.3.1 is a straightforward induction on the shape of the input formula and can be found below. It relies on the following Lemma 8.3.2 that shows how to turn a formula of the shape $(\mathsf{Q}{+}k)\overline{y}\,\psi$, where Q is ultimately periodic with period $p \geq 1$, into an equivalent Boolean combination of formulas using only threshold-counting (and modulo-counting with period p if $p \geq 2$).

The idea is to consider the characteristic sequence $\chi_{\mathsf{Q}} = \alpha\pi^{\omega}$ of Q, in which α, π are suitable words over the alphabet $\{0, 1\}$. The non-periodic part α can be expressed with threshold-counting using the existential quantifier. The periodic part π can be expressed by formulae using modulo-counting quantifiers with period p, each speaking about one position of π.

Lemma 8.3.2. *Let $U \subseteq U_{\text{all}}$, let $\mathsf{Q} \in U$ be ultimately periodic with period $p \geq 1$, and let*

$$\varphi \;:=\; (\mathsf{Q}{+}k)\overline{y}\,\psi$$

be a formula, where $\mathsf{Q} \in U$ is ultimately periodic with period $p \geq 1$, $k \geq 0$, $\overline{y}$ is a non-empty tuple of pairwise distinct variables, and ψ is a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}(D^U)_{\text{tpl}}$ with threshold $T \geq 0$.

There is an algorithm which computes, on input of φ, a formula from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\text{tpl}}$ that is equivalent to φ, that has the same quantifier rank and dimension as φ, and that has threshold $\leq \max\{||(\mathsf{Q}{+}k)||{-}2, T\}$.

The algorithm takes time in

$$||\varphi|| \cdot \mathcal{O}(||(\mathsf{Q}{+}k)||).$$

Proof. Let $U \subseteq U_{\text{all}}$, let $\mathsf{Q} \in U$ be ultimately periodic with period $p \geq 1$, let $\varphi \in \mathsf{FO}{+}\mathrm{un}\mathsf{T}(D^U)_{\text{tpl}}$, let $\overline{y}$ be a tuple of $m \geq 1$ distinct variables, and let $k \geq 0$.

Recall that $(\mathsf{Q}{+}k)$ is also ultimately periodic with period p and represented by a word $\alpha\#\pi$, where $n_0 := |\alpha|$ is the smallest offset and $|\pi| = p$, such that $\chi_{(\mathsf{Q}+k)} = \alpha\pi^\omega$.

In the following construction, we distinguish on whether $p = 1$ or $p \geq 2$. In both cases, a disjunction over an empty set will stand for the unsatisfiable formula $\exists\overline{y}\,\psi \wedge \neg\exists\overline{y}\,\psi$, and $\exists^{\geq 0}\overline{y}\,\psi$ will represent the tautological formula $\exists\overline{y}\,\psi \vee \neg\exists\overline{y}\,\psi$.

(Case 1) *If* $p = 1$, we only need threshold-counting quantifiers to express the quantifier $(\mathsf{Q}{+}k)$. We let S_0 the set of all $n \in (\mathsf{Q}{+}k)$ with $n < n_0$, and choose the formula

$$\begin{array}{ll} \bigvee_{n \in S_0} \exists^{=n}\overline{y}\,\psi & \text{if } \pi = 0, \text{ or} \\ \bigvee_{n \in S_0} \exists^{=n}\overline{y}\,\psi \;\;\vee\;\; \exists^{\geq n_0}\overline{y}\,\psi & \text{if } \pi = 1. \end{array}$$

(Case 2) *If* $p \geq 2$, we let $n_1 \in \mathbb{N}$ be the (unique) number in $[n_0, n_0 + p)$ that is divisible by p. Clearly, $(\mathsf{Q}{+}k)$ is also ultimately periodic with period p and offset n_1. Let

$$R \;:=\; \{r \in [0, p) \,:\, n_1 + r \in (\mathsf{Q}{+}k)\}.$$

It is now straightforward to verify that $(\mathsf{Q}{+}k)\overline{y}\,\psi$ is equivalent to the formula

$$\bigvee_{n \in S_1} \exists^{=n}\overline{y}\,\psi \;\;\vee\;\; \Bigg(\exists^{\geq n_1}\overline{y}\,\psi \;\;\wedge\;\; \bigvee_{r \in R} \exists^{\equiv r \bmod p}\overline{y}\,\psi \Bigg),$$

where S_1 is the set of all $n \in (\mathsf{Q}{+}k)$ with $n < n_1$.

In both cases, the resulting formula belongs to the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\mathrm{tpl}}$, has the same quantifier rank and the same dimension as $(\mathsf{Q}{+}k)\overline{y}\,\psi$ and, by the inequalities $n_0, n_1 < n_0 + p < ||(\mathsf{Q}{+}k)||$, threshold $\leq \max\{||(\mathsf{Q}{+}k)||{-}2, T\}$.

Time complexity. By construction, $|S_0|, |S_1| \leq n_1 < ||(\mathsf{Q}{+}k)||$. Furthermore, also $|R| \leq p < ||(\mathsf{Q}{+}k)||$. Observe that all the quantified subformulae in the constructed formula have size linear in $||\varphi||$. Thus, the algorithm takes time in

$$||\varphi|| \cdot \mathcal{O}(||(\mathsf{Q}{+}k)||).$$

This completes the proof of Lemma 8.3.2. $\square$

Proof of Lemma 8.3.1 using Lemma 8.3.2. Let $U \subseteq U_{\mathrm{all}}$ and let φ a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}$ with quantifier weight $w \geq 2$. The algorithm proceeds by an induction over the shape of φ, where the only size increasing step is the one for quantified subformulae of the shape $(\mathsf{Q}{+}k)\overline{y}\,\varphi'$ with $\mathsf{Q} \in U$, which, according to Lemma 8.3.2, increases the resulting formula by a factor in $\mathcal{O}(w)$. Thus the size of the formula $\tilde{\varphi}$, which the algorithm computes, and the time needed for its construction is in

$$\mathcal{O}(||\varphi||) \cdot \mathcal{O}(w)^q.$$

Since each threshold-counting quantifier $(\exists{+}k)$ already present in φ has $k < w$, it can be shown straightforwardly along the course of the induction that $\tilde{\varphi}$ has threshold $< w$. This completes the proof of Lemma 8.3.1. $\square$

8.3.2 From Modulo-Counting to Ultimately Periodic Quantifiers

In the following, it is shown how to turn a formula of the shape $(\mathsf{D}_p{+}k)y\,\varphi$ with period $p \geq 2$ into a Boolean combination of formulae using only threshold-counting and arbitrary ultimately periodic counting quantifiers with the same period p.

Before doing this, we prove the following lemma that will turn out to be central in this translation. Intuitively, it tells us the following: Suppose that the quantifier Q is ultimately periodic with period $p \geq 1$ and offset $n_0 \geq 0$. Then, for any number $n \geq n_0$ we can decide whether n is congruent n_0 modulo p just by looking at the p positions in the characteristic sequence of Q that follow on n.

Lemma 8.3.3. *Let $\alpha, \beta, \pi \in \{0,1\}^*$ such that π is primitive of length $p \geq 1$ and β is a prefix of $\alpha\pi^\omega$ of length at least $|\alpha|$. Then,*

$$|\alpha| \;\equiv\; |\beta| \mod p \quad \textit{iff} \quad \beta\pi \textit{ is a prefix of } \alpha\pi^\omega\,.$$

Proof. We prove the two directions of the equivalence.

"Only if" direction. Suppose $|\beta| - |\alpha|$ is a multiple of $p = |\pi|$, that is, there is an $i \geq 0$ such that $|\beta| - |\alpha| = ip$. Since β is a prefix of $\alpha\pi^\omega$, in particular $\beta = \alpha\pi^i$. Hence, also $\beta\pi = \alpha\pi^{i+1}$ is a prefix of $\alpha\pi^\omega$.

"If" direction. Suppose now that $\beta\pi$ is a prefix of $\alpha\pi^\omega$. Let $i \in \mathbb{N}$ be maximal such that $\alpha\pi^i$ is a prefix of $\beta\pi$. Such an $i \geq 0$ exists since $\alpha = \alpha\pi^0$ is a prefix of β.

The following claim shows that $|\beta| - |\alpha|$ is a multiple of p and, this way, completes the proof of Lemma 8.3.3.

Claim 1. *$\alpha\pi^i = \beta\pi$.*

Proof of Claim 1. Towards a contradiction, assume that $\alpha\pi^i$ is a proper prefix of $\beta\pi$, that is, there exists a non-empty word $u \in \{0,1\}^*$ of length $< p$ such that $\alpha\pi^i u = \beta$.

Since $\beta\pi$ and $\alpha\pi^{i+1}$ both are prefixes of $\alpha\pi^\omega$ and since $|\beta\pi| < |\alpha\pi^{i+1}|$, there exists $v \in \{0,1\}^*$ with $\beta\pi v = \alpha\pi^{i+1}$. Hence $\alpha\pi^{i+1} = \beta\pi v = \alpha\pi^i uv$, which implies that $uv = \pi$.

Moreover, $\beta\pi vu = \alpha\pi^{i+1}u$ is a prefix of $\alpha\pi^\omega$. Note that $(\alpha\pi^\omega)[n] = (\alpha\pi^\omega)[n{+}p]$ for all $n \geq |\alpha|$ and therefore in particular for all $n \geq |\beta|$. Since $\beta\pi$ is a prefix of $\alpha\pi^\omega$, this implies $\alpha\pi^\omega = \beta\pi^\omega$, that is, $\beta\pi vu$ is a prefix of $\beta\pi^\omega$. Hence vu is a prefix of π^ω of length $|vu| = |uv| = |\pi|$, that is, $vu = \pi$.

Thus, we have $uv = \pi = vu$. We use the following proposition, adapted from [Lot84, Proposition 1.3.2]:

Proposition 8.3.4. *For all non-empty words $u, v \in \{0,1\}^*$, it holds that*

$$uv = vu \quad \textit{iff} \quad \textit{there is a word } w \in \{0,1\}^* \textit{ such that } u, v \in w^*.$$

Let $w \in \{0,1\}^*$ such that $u, v \in w^*$ and therefore $\pi \in w^*$. Since π is primitive, this implies $w = \pi$. Since $|u| < |\pi|$ and $u \in \pi^*$, we obtain $u = \varepsilon$. This is a contradiction to the assumption that u is non-empty, and completes the proof of Claim 1 and Lemma 8.3.3. □

We now turn the observation of Lemma 8.3.3 into a construction for the desired formula.

Lemma 8.3.5. *Let $U \subseteq U_{\text{all}}$, let $\mathsf{Q} \in U$ be ultimately periodic with period $p \geq 2$, and let*

$$\varphi \;:=\; \exists^{\equiv r \bmod p} y\, \psi$$

for $r \in [0, p)$ and a formula ψ from $\mathsf{FO}+\mathrm{un}\mathsf{C}(U)_{\text{tpl}}$.

There is an algorithm which, on input of φ and Q, computes a Boolean combination of formulae from $\mathsf{FO}+\mathrm{un}\mathsf{C}(U)_{\text{tpl}}$ of the shape

$$(\mathsf{Q}{+}\ell) y\, \psi \quad \textit{and} \quad \exists^{>\ell} y\, \psi$$

with $||(\mathsf{Q}{+}\ell)||, ||\exists^{>\ell}|| < ||\mathsf{Q}|| + p$ that is equivalent to φ.

Furthermore, the algorithm takes time in

$$\mathcal{O}(||\varphi||) \cdot (||\mathsf{Q}|| + p)^2.$$

Proof. Let $U \subseteq U_{\text{all}}$ and let $\mathsf{Q} \in U$ be ultimately periodic with period $p \geq 2$. Furthermore, let $\varphi := \exists^{\equiv r \bmod p} y\, \psi$ for an $r \in [0, p)$ and a formula ψ from $\mathsf{FO}+\mathrm{un}\mathsf{C}(U)_{\text{tpl}}$.

Let $n_0 \geq 0$ be the minimal offset of Q and let furthermore α be the shortest prefix of χ_{Q} of length $n_1 \geq \max\{n_0, r\}$ with $|\alpha| \equiv r \mod p$. Then there exists a primitive word π of length p with $\chi_{\mathsf{Q}} = \alpha\pi^\omega$.

Let $\pi_1, \pi_2, \ldots, \pi_p \in \{0, 1\}$ such that $\pi = \pi_p \cdots \pi_2 \pi_1$. It is straightforward to see that for all $n \in \mathbb{N}$ with $n \geq |\alpha\pi|$,

$$\begin{array}{ll} & \chi_{\mathsf{Q}}[n{-}p, n) \;=\; \pi \\[1ex] \text{iff} & n{-}i \in \mathsf{Q} \text{ for each } i \in [1, p] \text{ with } \pi_i = 1, \text{ and} \\ & n{-}i \notin \mathsf{Q} \text{ for each } i \in [1, p] \text{ with } \pi_i = 0 \\[1ex] \text{iff} & n \in \mathsf{Q}{+}i \text{ for each } i \in [1, p] \text{ with } \pi_i = 1, \text{ and} \\ & n \notin \mathsf{Q}{+}i \text{ for each } i \in [1, p] \text{ with } \pi_i = 0. \end{array}$$

By Lemma 8.3.3, the formula $\exists^{\equiv r \bmod p} y\, \varphi$ is equivalent to the formula

$$\begin{array}{ll} & \bigvee_{n \in S} \exists^{=n} y\, \psi \\ \vee & \left(\exists^{\geq n_1 + p - 1} y\, \psi \quad \wedge \bigwedge_{\substack{i \in [1,p]:\\ \pi_i = 1}} (\mathsf{Q}{+}i) y\, \psi \quad \wedge \bigwedge_{\substack{j \in [1,p]:\\ \pi_j = 0}} \neg\, (\mathsf{Q}{+}j) y\, \psi \right), \end{array} \tag{1}$$

where S is the set of all $n \in \exists^{\equiv r \bmod p}$ with $n < |\alpha\pi|$.

Observe that $n_1 < n_0 + p$ and thus, $\alpha\pi$ has length less than $n_0 + 2p$. Therefore, each of the quantifiers that explicitly occur in Formula (1) has size less than

$$||\mathsf{Q}|| + p.$$

Using this, it is straightforward to see that Formula (1) can be computed in time

$$\mathcal{O}(||\varphi||) \cdot (||\mathsf{Q}|| + p)^2.$$

This completes the proof of Lemma 8.3.5. □

8.4 Hanf Normal Form

In Chapter 3 and Section 7.3 we have seen that the logics $\mathsf{FO}+\mathrm{unM}(D)$ and $\mathsf{FO}+\mathrm{unM}(D)_{\mathrm{tpl}}$, for all $D \subseteq D_{\mathrm{all}}$, permit Hanf normal form, and that the corresponding HNF-formulae can also be computed effectively and, in particular, in worst-case optimal 3-fold exponential time (for degree bounds ≥ 3).

In this section, we build on these results to provide complete answers to Question (1) and Question (2) from Section 3.1. More precisely, we show the following characterisation of all logics $\mathsf{FO}+\mathrm{unC}(C)_{\mathrm{tpl}}$ with $C \subseteq C_{\mathrm{all}}$ that permit Hanf normal form. Note that the same characterisation also holds for the logics $\mathsf{FO}+\mathrm{unC}(C)$ with $C \subseteq C_{\mathrm{all}}$, since HNF-formulae only have dimension one.

Theorem 8.4.1. *For every set $C \subseteq C_{\mathrm{all}}$, the following equivalence holds:*

$\mathsf{FO}+\mathrm{unC}(C)_{\mathrm{tpl}}$ *permit Hanf normal form*

iff *every quantifier in C is ultimately periodic.*

Proof. Let $C \subseteq C_{\mathrm{all}}$.

For the "if" direction, suppose that all quantifiers in C are ultimately periodic. We have to show that for each relational signature σ and each formula φ from $\mathsf{FO}+\mathrm{unC}(C)_{\mathrm{tpl}}[\sigma]$, there is a d-equivalent HNF-formulae for every degree bound $d \geq 0$.

To this aim, Theorem 8.4.2 further down below actually provides an elementary algorithm for the construction of such HNF-formulae.[2]

[2] Observe that for any formula φ, every d-equivalent HNF-formula is also d'-equivalent to φ for every degree bound $d' < d$.

For the "only if" direction, suppose that C contains a quantifier S that is *not* ultimately periodic. Let P be a unary relation symbol. We will show that there is a sentence from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)[P]$ (and thus, from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)_{\mathrm{tpl}}[P]$), for which there is no d-equivalent HNF-formula in $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)[P]$ for any degree bound $d \geq 0$.

Observe that, since P is unary, every (P)-structure has degree 0. In every structure $\mathcal{A}$ over the signature (P), the $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)[P]$-sentence $\mathsf{S}y\, y{=}y$ expresses that $|A| \in \mathsf{S}$. Towards a contradiction, assume that there is a HNF-sentence ψ in $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)[P]$ that is equivalent to $\mathsf{S}y\, y{=}y$.

Since P is unary, any σ_P-type of any radius with one centre consists of its centre, only. Consequently, every sphere-formula $\mathrm{sph}_\tau(y)$, where τ is a (P)-type with one centre, is either equivalent to the formula $P(y)$ or to the formula $\neg P(y)$. In particular, this means that the HNF-sentence ψ is equivalent to a Boolean combination of sentences of the shape

$$(\mathsf{Q}{+}\ell)y\, P(y) \quad \text{or} \quad (\mathsf{Q}{+}\ell)y\, \neg P(y)$$

with $\mathsf{Q} \in C \cup \{\exists\}$ and $\ell \geq 0$. However, this is a contradiction to Lemma 8.2.1. $\square$

In the following section, we show how HNF-formulae for formulae from logics $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}$ with $U \subseteq U_{\mathrm{all}}$ can be computed effectively. Afterwards, a locality theorem for $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}$ in the manner of Nurmonen's theorem [Nur00] will be presented. The section is concluded by a model-checking algorithm for $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}$.

8.4.1 Constructing Hanf Normal Form

In this subsection, we prove the following result:

Theorem 8.4.2. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *a relational signature σ, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}[\sigma]$ with $U \subseteq U_{\mathrm{all}}$,*

computes a HNF*-formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)[\sigma]$ that is d-equivalent to $\varphi(\overline{x})$.*

Let $w \geq 2$ and $n, q \geq 0$ be the quantifier weight, the number of free variables, and the quantifier rank of $\varphi(\overline{x})$, respectively.

The computed formula $\psi(\overline{x})$ has locality radius $\leq 4^q$ and quantifier weight

$$< \ 2w + (n{+}q) \cdot \nu_d(4^q).$$

Moreover, the algorithm constructs $\psi(\overline{x})$ in time

$$2^{\left(||\varphi|| \cdot 2^{q \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}.$$

Remark 8.4.3. Clearly, $w, n, q < ||\varphi||$. Furthermore, suppose that σ only contains relation symbols that actually occur in $\varphi(\overline{x})$ and thus, $||\sigma|| < ||\varphi||$. Then, the algorithm of Theorem 8.4.2 takes 3-fold exponential time

$$2^{d^{2^{\mathcal{O}(||\varphi||)}}}$$

in the size of the input formula for degree bounds $d \geq 3$, and, for $d = 2$, 2-fold exponential time

$$2^{2^{\mathrm{poly}(||\varphi||)}}.$$

Proof. Let $d \geq 2$ be a degree bound, let σ be a relational signature, and let $U \subseteq U_{\mathrm{all}}$. Furthermore, let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}[\sigma]$ with $n \geq 0$ free variables.

The algorithm proceeds in the following three steps:

(Step 1) The algorithm of Lemma 8.3.1 constructs a formula $\tilde{\varphi}(\overline{x})$ from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\mathrm{tpl}}[\sigma]$ that is equivalent to $\varphi(\overline{x})$. The size of $\tilde{\varphi}(\overline{x})$ and the time to construct the formula are bounded by

$$\mathcal{O}(||\varphi||) \cdot \mathcal{O}(w)^q, \tag{1}$$

where $w \geq 2$ and $q \geq 0$ are the quantifier weight and the quantifier rank of $\varphi(\overline{x})$. Furthermore, the threshold and the maximum period of $\tilde{\varphi}(\overline{x})$ are $< w$, and $\tilde{\varphi}$ has the same quantifier rank as $\varphi(\overline{x})$.

(Step 2) On input of d, σ, and $\tilde{\varphi}(\overline{x})$, the algorithm of Theorem 7.3.1 computes a HNF-formula $\tilde{\psi}(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)[\sigma]$ that is d-equivalent to $\tilde{\varphi}(\overline{x})$ and thus, also d-equivalent to $\varphi(\overline{x})$. Using the upper bounds on the size, the threshold, and the maximum period of $\tilde{\varphi}(\overline{x})$, this takes time in

$$\begin{aligned} & 2^{\left(\mathcal{O}(||\varphi||) \cdot \mathcal{O}(w)^q \cdot 2^{q \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}} \\ \subseteq \quad & 2^{\left(||\varphi|| \cdot 2^{q \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}. \end{aligned} \tag{2}$$

Furthermore, by Theorem 7.3.1, $\tilde{\psi}(\overline{x})$ has threshold $< w + (n{+}q) \cdot \nu_d(4^q)$ and locality radius $\leq 4^q$.

(Step 3) We apply the algorithm of Lemma 8.3.5 to each counting-sentence of the shape $\chi := \exists^{\equiv r \bmod p} y\ \mathrm{sph}_\tau(y)$ in $\tilde{\psi}(\overline{x})$ and the corresponding quantifier $\mathsf{Q} \in U$ of period p. By the transformations in the previous steps, we can assume that Q already occurs in $\varphi(\overline{x})$ and thus, $||\mathsf{Q}|| \leq w$ and, in particular, $||\mathsf{Q}|| + p < 2w$. For each such counting-sentence, the algorithm of Lemma 8.3.5 takes time in

$$\mathcal{O}(||\chi||) \cdot (2w)^2$$

and results in an equivalent HNF-formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)[\sigma]$ with quantifier weight $< 2w$.

Since the number and size of such counting-sentences is bounded by the size of $\tilde{\psi}(\overline{x})$, it takes time in

$$\begin{aligned} & \mathcal{O}(w)^2 \cdot \Big(2^{\left(||\varphi|| \cdot 2^{q \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}\Big)^2 \\ \subseteq \quad & 2^{\left(||\varphi|| \cdot 2^{q \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}} \end{aligned} \tag{3}$$

to obtain a HNF-formula $\psi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)[\sigma]$ that is equivalent to $\tilde{\psi}(\overline{x})$ and thus, d-equivalent to $\varphi(\overline{x})$. Furthermore, by taking the threshold of the HNF-formula $\tilde{\psi}(\overline{x})$ into account, we know that $\psi(\overline{x})$ has quantifier weight

$$< \ \max\{2w, w + (n{+}q) \cdot \nu_d(4^q) + 2\} \ < \ 2w + (n{+}q) \cdot \nu_d(4^q).$$

Adding up Estimates (1) to (3), we can conclude that the algorithm takes time in

$$2^{\left(||\varphi|| \cdot 2^{q \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}}$$

to compute $\psi(\overline{x})$ from $\varphi(\overline{x})$. This completes the proof of Theorem 8.4.2. $\square$

8.4.2 A Locality Theorem for Ultimately Periodic Quantifiers

In this section, we generalise the locality theorem of Section 7.3 from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ to the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$. More precisely, we prove the following:

Theorem 8.4.4. *Let σ be a relational signature and let $d \geq 2$ be a degree bound. Furthermore, let $w \geq 2$, $n, q \geq 0$, and $M \geq 1$.*

Suppose that $\mathcal{A}$ and $\mathcal{B}$ are d-bounded σ-structures and $\overline{a} \in A^n$, $\overline{b} \in B^n$, such that the following Conditions (1) to (3) are satisfied for $r := 4^q$:

(1) $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \;\cong\; \mathcal{N}_r^{\mathcal{B}}(\overline{b})$.

For every type $\tau \in \mathfrak{T}_r^{d,\sigma}(1)$,

(2) $|\tau(\mathcal{A})| \;\equiv\; |\tau(\mathcal{B})| \mod M$, *and*

(3) either $|\tau(\mathcal{A})| \;=\; |\tau(\mathcal{B})|$ *or*

$$|\tau(\mathcal{A})|, |\tau(\mathcal{B})| \;\geq\; w + (n{+}q) \cdot \nu_d(r).$$

Then, for every tuple $\overline{x}$ *of* n *pairwise distinct variables, for every formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}[\sigma]$ *with quantifier weight* $\leq w$*, quantifier rank* $\leq q$*, and such that* M *is a common multiple of the periods of all ultimately periodic counting quantifiers that occur in* $\varphi(\overline{x})$*,*

$$\mathcal{A} \;\models\; \varphi[\overline{a}] \quad \textit{iff} \quad \mathcal{B} \;\models\; \varphi[\overline{b}].$$

Proof. Let σ be a relational signature and let $d \geq 2$ be a degree bound. Furthermore, let $w \geq 2$, $n, q \geq 0$, and $M \geq 1$. Suppose that $\mathcal{A}$ and $\mathcal{B}$ are d-bounded σ-structures and $\overline{a} \in A^n$, $\overline{b} \in B^n$, such that Conditions (1) to (3) of Theorem 8.4.4 are satisfied.

Consider a tuple $\overline{x}$ of n pairwise distinct variables, and a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}[\sigma]$ with quantifier weight $\leq w$, quantifier rank $\leq q$, where M is a common multiple of the periods of all ultimately periodic counting quantifiers occurring in $\varphi(\overline{x})$. Let $U \subseteq U_{\mathrm{all}}$ consist of precisely the ultimately periodic counting quantifiers that occur in φ.

By Lemma 8.3.1, $\varphi(\overline{x})$ is equivalent to a formula $\tilde{\varphi}(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\mathrm{tpl}}[\sigma]$ with the same dimension and quantifier rank, and with threshold $< w$. Furthermore, M is also a common multiple of the periods of all modulo-counting quantifiers occurring in $\tilde{\varphi}(\overline{x})$. In particular, we know by Theorem 7.3.3 that

$$\mathcal{A} \;\models\; \tilde{\varphi}[\overline{a}] \quad \text{iff} \quad \mathcal{B} \;\models\; \tilde{\varphi}[\overline{b}].$$

Thus, since $\varphi(\overline{x})$ and $\tilde{\varphi}(\overline{x})$ are equivalent, also

$$\mathcal{A} \;\models\; \varphi[\overline{a}] \quad \text{iff} \quad \mathcal{B} \;\models\; \varphi[\overline{b}].$$

This completes the proof of Theorem 8.4.4. □

8.4.3 Model-Checking

In this section, we generalise the model-checking algorithm of Section 7.3 from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ to $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$. That is, we prove the following:

Theorem 8.4.5. *There is an algorithm which, on input of*

- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ where the tuple $\overline{x}$ consists of the $n \geq 0$ free variables of $\varphi(\overline{x})$,*
- *a finite σ-structure $\mathcal{A}$ (where σ consists of precisely the relation symbols that occur in φ), and a tuple $\overline{a} \in A^n$,*

decides whether $\mathcal{A} \models \varphi[\overline{a}]$.

This algorithm takes time in

$$2^{\left(||\varphi||\cdot 2^{q\cdot(\log w)^2}\cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}} \cdot ||\mathcal{A}||$$

where $w \geq 2$ and $q \geq 0$ are the quantifier weight and the quantifier rank of $\varphi(\overline{x})$.

Remark 8.4.6. Since $w, q, ||\sigma|| < ||\varphi||$, the algorithm of Theorem 8.4.5 takes 3-fold exponential time in the size of $\varphi(\overline{x})$ for every σ-structure $\mathcal{A}$ with degree ≥ 3, and 2-fold exponential time for every σ-structure $\mathcal{A}$ with degree ≤ 2 (and linear time in the size of $\mathcal{A}$).

Proof of Theorem 8.4.5. Let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}[\sigma]$ with $U \subseteq U_{\mathrm{all}}$, where $\overline{x}$ are the $n \geq 0$ free variables of φ and where σ consists of precisely the relation symbols that occur in $\varphi(\overline{x})$. Furthermore, let $\mathcal{A}$ be a σ-structure and $\overline{a} \in A^n$.

The algorithm proceeds in the following two steps:

(Step 1) The algorithm of Lemma 8.3.1 constructs a formula $\tilde{\varphi}(\overline{x})$ from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\mathrm{tpl}}[\sigma]$ that is equivalent to $\varphi(\overline{x})$. This takes time in

$$\mathcal{O}(||\varphi||) \cdot \mathcal{O}(w)^q, \tag{1}$$

where $w \geq 2$ and $q \geq 0$ are the quantifier weight and the quantifier rank of $\varphi(\overline{x})$. By Lemma 8.3.1, the threshold and the maximum period of $\tilde{\varphi}(\overline{x})$ are $< w$, and $\tilde{\varphi}(\overline{x})$ has the same quantifier rank as $\varphi(\overline{x})$.

(Step 2) On input of $\tilde{\varphi}(\overline{x})$, $\mathcal{A}$, and $\overline{a}$, the algorithm of Theorem 7.3.4 decides whether $\mathcal{A} \models \tilde{\varphi}[\overline{a}]$ and thus, whether $\mathcal{A} \models \varphi[\overline{a}]$. Using the upper bounds of Step (1), this takes time in

$$\begin{aligned} & 2^{\left(\mathcal{O}(||\varphi||)\cdot\mathcal{O}(w)^q\cdot 2^{q\cdot(\log w)^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}} \cdot ||\mathcal{A}|| \\ \subseteq \quad & 2^{\left(||\varphi||\cdot 2^{q\cdot(\log w)^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}} \cdot ||\mathcal{A}||. \end{aligned} \qquad (2)$$

Altogether we obtain from Estimate (1) and Estimate (2) that the algorithm terminates in time

$$2^{\left(||\varphi||\cdot 2^{q\cdot(\log w)^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma||)}} \cdot ||\mathcal{A}||.$$

This completes the proof of Theorem 8.4.5. $\square$

8.5 Feferman-Vaught Decompositions

In this section, we use the construction of HNF-formulae for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$, provided by Section 8.4, to obtain Feferman-Vaught decompositions for this logic. The algorithms for the construction of $\oplus$-decompositions, decompositions defined by transductions and $\otimes$-decompositions, described below, rely on the corresponding algorithms in Section 7.4.

Furthermore, we show, similarly to the case of Hanf normal form in Section 8.4, that only logics with only ultimately periodic counting quantifiers allow the construction of $\oplus$-decompositions. Thus, the algorithms presented in this section can not be further extended in terms of the allowed unary counting quantifiers of the input formulae.

For a more precise statement, suppose that L is one of the logics $\mathsf{FO}{+}\mathrm{un}\mathsf{T}$, $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)$ with $D \subseteq D_{\mathrm{all}}$, or $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)$ with $C \subseteq C_{\mathrm{all}}$, or one of the corresponding tuple-counting logics $\mathsf{FO}{+}\mathrm{un}\mathsf{T}_{\mathrm{tpl}}$, $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)_{\mathrm{tpl}}$, or $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)_{\mathrm{tpl}}$, defined in Section 2.4.2. We say:

Definition 8.5.1. L *permits $\oplus$-decompositions* if for each degree bound $d \geq 0$, every relational signature σ, each $s \geq 1$ and every $\mathsf{L}[\sigma_s]$-formula $\varphi(\overline{x})$, there is an s-ary $\oplus$-decomposition for $\varphi(\overline{x})$ over $\mathsf{L}[\sigma]$ on $\mathfrak{C}^{d,\sigma}$.

By Chapter 5 and Section 7.4, we already know that the logics $\mathsf{FO}{+}\mathrm{un}\mathsf{T}$ and $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D)$ for all $D \subseteq D_{\mathrm{all}}$ permit $\oplus$-decompositions and that the same holds for $\mathsf{FO}{+}\mathrm{un}\mathsf{T}_{\mathrm{tpl}}$ and $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}(D)$. Here, we provide the following characterisation:

Theorem 8.5.2. *For every set $C \subseteq C_{\text{all}}$, the following equivalence holds:*

$\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)_{\text{tpl}}$ *permits $\oplus$-decompositions*

iff *every quantifier in C is ultimately periodic.*

Proof. Let $C \subseteq C_{\text{all}}$.

For the "if" direction, suppose that all quantifiers in C are ultimately periodic. For each degree bound $d \geq 0$ and every relational signature σ, each $s \geq 1$, and every formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)_{\text{tpl}}[\sigma_s]$, the algorithm of Theorem 8.5.3 further down below computes an s-ary $\oplus$-decomposition over $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)[\sigma]$ on the class of d-bounded σ-structures.[3]

For the "only if" direction, suppose that C contains a quantifier S that is *not* ultimately periodic. We proceed in a similar fashion as in the proof of the "only if" direction of Theorem 8.4.1.

In the following, we denote by $\mathfrak{C}$ the class of all finite structures over the empty signature $\emptyset$. All structures in $\mathfrak{C}$ are sets of isolated elements and thus have degree 0.

Note that, in any structure $\mathcal{A} \in \mathfrak{C}$, the $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)[\emptyset]$-sentence $\varphi := \mathsf{S}y\, y{=}y$ expresses that $|A| \in \mathsf{S}$. Towards a contradiction, assume that there is a 2-ary $\oplus$-decomposition $\Delta = (\beta, \Delta_1, \Delta_2)$ for φ over $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)_{\text{tpl}}[\emptyset]$ on $\mathfrak{C}$. In the following, we show that such a $\oplus$-decomposition leads to a contradiction to Lemma 8.2.1.

All formulae in Δ_1 and Δ_2 are sentences from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(C)_{\text{tpl}}[\emptyset]$. For every $i \in \{1,2\}$ and each propositional symbol $X_{i,\delta}$ with $\delta \in \Delta_i$ that occurs in β, we define a unary counting quantifier $\mathsf{Q}_{i,\delta} \subseteq \mathbb{N}$ such that

$$\mathsf{Q}_{i,\delta} \;:=\; \{|A| \,:\, \mathcal{A} \in \mathfrak{C} \text{ and } \mathcal{A} \models \delta\}.$$

Let P be a unary relation symbol. We replace each propositional symbol $X_{i,\delta}$ in β with the sentence

$$\begin{array}{ll} \mathsf{Q}_{i,\delta}\, y\, P(y) & \text{if } i = 1, \text{ and} \\ \mathsf{Q}_{i,\delta}\, y\, \neg P(y) & \text{if } i = 2. \end{array}$$

and call the resulting $\mathsf{FO}{+}\mathrm{un}\mathsf{C}[P]$-sentence ψ. On almost all σ_P-structures, ψ is equivalent to φ:

[3]Note that the algorithm of Theorem 8.5.3 only takes degree bounds $d \geq 2$ as an input. This does not pose any problem here, since every $\oplus$-decomposition on 2-bounded σ-structures is also a $\oplus$-decomposition on d-bounded σ-structures for $d < 2$.

Claim 1. *For every (P)-structure $\mathcal{A}$ where neither $P^{\mathcal{A}} = A$ nor $P^{\mathcal{A}} = \emptyset$,*

$$\mathcal{A} \models \psi \quad \textit{iff} \quad \mathcal{A} \models \varphi.$$

Proof of Claim 1. Let $\mathcal{A}$ be a (P)-structure with $\emptyset \subset P^{\mathcal{A}} \subset A$, and let $\mathcal{A}_1, \mathcal{A}_2 \in \mathfrak{C}$ be the $\emptyset$-structures with universes $A_1 = P^{\mathcal{A}}$ and $A_2 = A \setminus P^{\mathcal{A}}$, respectively (note that we had to make the restriction on the set $P^{\mathcal{A}}$ to be able to define these structures properly).

Since Δ is a 2-ary $\oplus$-decomposition for φ on $\mathfrak{C}$, we know that

$$\mathcal{A}_1 \oplus \mathcal{A}_2 \models \varphi \quad \text{iff} \quad \mathcal{A}_1, \mathcal{A}_2 \models \Delta.$$

In order to show that

$$\mathcal{A}_1, \mathcal{A}_2 \models \Delta \quad \text{iff} \quad \mathcal{A} \models \psi,$$

we show that for every propositional symbol $X_{i,\delta}$ that occurs in β,

$$\begin{array}{llll} \mathcal{A}_1 \models \delta & \text{iff} & \mathcal{A} \models \mathsf{Q}_{1,\delta}\, y\, P(y) & \text{if } i = 1, \text{ and} \\ \mathcal{A}_2 \models \delta & \text{iff} & \mathcal{A} \models \mathsf{Q}_{2,\delta}\, y\, \neg P(y) & \text{if } i = 2. \end{array}$$

We only prove the case of $i = 1$. The argumentation for $i = 2$ is analogous. Let $X_{1,\delta}$ be a propositional symbol with $\delta \in \Delta_1$ that occurs in β. Then, the following equivalences holds:

$$\begin{array}{lrcll} & \mathcal{A}_1 & \models & \delta & \\ \text{iff} & |A_1| & \in & \mathsf{Q}_{1,\delta} & \text{(by definition of } \mathsf{Q}_{1,\delta}) \\ \text{iff} & |P^{\mathcal{A}}| & \in & \mathsf{Q}_{1,\delta} & \text{(by construction of } \mathcal{A}_1) \\ \text{iff} & \mathcal{A} & \models & \mathsf{Q}_{1,\delta}\, y\, P(y). & \end{array}$$

This completes the proof of Claim 1.

We now use the sentence ψ to construct a sentence that is equivalent to φ on *all* σ_P-structures $\mathcal{A}$. To this aim, we have to handle the special cases that $P^{\mathcal{A}} = A$ and that $P^{\mathcal{A}} = \emptyset$. Clearly, we can choose

$$\Big(\exists y\, P(y) \land \exists y\, \neg P(y) \land \psi\Big) \lor \Big(\neg \exists y\, \neg P(y) \land \mathsf{S} y\, P(y)\Big) \lor \Big(\neg \exists y\, P(y) \land \mathsf{S} y\, \neg P(y)\Big).$$

However, we know by Lemma 8.2.1 that, since S is not ultimately periodic, such a sentence can not exist. This leads to the desired contradiction and thus completes the proof of Theorem 8.5.2. $\square$

8.5.1 Decompositions with respect to Disjoint Sums

In this section, we generalise the algorithm of Theorem 7.4.1 to formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$. More precisely, we show the following result:

Theorem 8.5.3. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$*,*
- *a relational signature* σ*,*
- *an arity* $s \geq 1$*, and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}[\sigma_s]$ *with* $U \subseteq U_{\mathrm{all}}$*,* $n := |\overline{x}|$ *free variables, quantifier weight* $w \geq 2$*, and quantifier rank* $q \geq 0$*,*

computes an s*-ary* $\oplus$*-decomposition* $(\beta, \Delta_1, \ldots, \Delta_s)$ *for* $\varphi(\overline{x})$ *over* $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)[\sigma]$ *on the class of* d*-bounded* σ*-structures, where all formulae in the sets* $\Delta_1, \ldots, \Delta_s$ *are* HNF*-formulae with quantifier weight* $< 2w + (n{+}q) \cdot \nu_d(4^q)$*.*

Furthermore, the algorithm computes Δ *in time*

$$2^{\left(||\varphi|| \cdot 2^{q \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}}.$$

Remark 8.5.4. Suppose that σ only contains relation symbols that actually occur in $\varphi(\overline{x})$. Recall that $w, q < ||\varphi||$. Then, the algorithm takes 3-fold exponential time

$$2^{d^{s \cdot 2^{\mathcal{O}(||\varphi||)}}}$$

in the size of φ for $d = 3$, and, for $d = 2$, 2-fold exponential time

$$2^{2^{s \cdot \mathrm{poly}(||\varphi||)}}.$$

Proof. Let $d \geq 2$ be a degree bound, let σ be a relational signature, and let $s \geq 1$. Furthermore, let $U \subseteq U_{\mathrm{all}}$ and let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}[\sigma_s]$ with $n := |\overline{x}|$ free variables, quantifier weight $w \geq 2$, and quantifier rank $q \geq 0$. The algorithm proceeds as follows:

(Step 1) The algorithm of Lemma 8.3.1 constructs a formula $\tilde{\varphi}(\overline{x})$ from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\mathrm{tpl}}[\sigma_s]$ that is equivalent to $\varphi(\overline{x})$. The size of $\tilde{\varphi}(\overline{x})$ and the time to construct the formula are bounded by

$$\mathcal{O}(||\varphi||) \cdot \mathcal{O}(w)^q \tag{1}$$

Furthermore, the threshold and the maximum period of $\tilde{\varphi}(\overline{x})$ are $< w$, and $\tilde{\varphi}(\overline{x})$ has the same quantifier rank as $\varphi(\overline{x})$.

(Step 2) On input of d, σ, s, and $\tilde{\varphi}(\overline{x})$, the algorithm of Theorem 7.4.1 computes an s-ary $\oplus$-decomposition $\tilde{\Delta} = (\tilde{\beta}, \tilde{\Delta}_1, \ldots, \tilde{\Delta}_s)$ for $\tilde{\varphi}(\overline{x})$ (and thus, for $\varphi(\overline{x})$) over $\mathsf{FO}{+}\mathrm{unM}(D^U)[\sigma]$ on the class of d-bounded σ-structures. In particular, all formulae in the sets $\tilde{\Delta}_1, \ldots, \tilde{\Delta}_s$ are HNF-formulae with threshold $< w + (n{+}q) \cdot \nu_d(4^q)$.

Since $\tilde{\varphi}(\overline{x})$ has threshold and maximum period $< w$, this takes time in

$$\begin{aligned} & 2^{\left(\mathcal{O}(||\varphi||)\cdot\mathcal{O}(w)^q\cdot 2^{q\cdot(\log w)^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}} \\ \subseteq\ & 2^{\left(||\varphi||\cdot 2^{q\cdot(\log w)^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}}. \end{aligned} \tag{2}$$

(Step 3) We apply the algorithm of Lemma 8.3.5 to each counting-sentence of the shape $\chi := \exists^{\equiv r \bmod p} y\ \mathrm{sph}_\tau(y)$ in each of the formulae of the sets $\tilde{\Delta}_1, \ldots, \tilde{\Delta}_s$ and the corresponding quantifier $\mathsf{Q} \in U$ of period p. By the transformations in the previous steps, we can assume that Q already occurs in $\varphi(\overline{x})$ and thus, $||\mathsf{Q}|| \leq w$ and, in particular, $||Q|| + p < 2w$. For each such counting-sentence, the algorithm of Lemma 8.3.5 takes time in $\mathcal{O}(||\chi||) \cdot (2w)^2$ and results in an equivalent HNF-formula from $\mathsf{FO}{+}\mathrm{unC}(U)[\sigma]$ with quantifier weight $< 2w$.

Since the number and size of such counting-sentences is bounded by the size of $\tilde{\Delta}$, it takes time in

$$\begin{aligned} & \mathcal{O}(w)^2 \cdot \left(2^{\left(||\varphi||\cdot 2^{q\cdot(\log w)^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}}\right)^2 \\ \subseteq\ & 2^{\left(||\varphi||\cdot 2^{q\cdot(\log w)^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}} \end{aligned} \tag{3}$$

to obtain an s-ary $\oplus$-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ for $\varphi(\overline{x})$ over $\mathsf{FO}{+}\mathrm{unC}(U)[\sigma]$ on the class of d-bounded σ-structures, where all formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF-formulae with quantifier weight less than $2w + (n{+}q) \cdot \nu_d(4^q)$.

Adding up Estimates (1) to (3), we see that altogether, the time required for the construction of Δ is in

$$2^{\left(||\varphi||\cdot 2^{q\cdot(\log w)^2}\cdot\nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}}.$$

This completes the proof of Theorem 8.5.3. $\square$

8.5.2 Decompositions with respect to Transductions and Direct Products

The following two results, which extend the algorithms of Theorem 7.4.3 and Theorem 7.4.5 to formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$, can be proven in a completely analogous way to Theorem 8.5.3, just by replacing the application of Theorem 7.4.1 in the proof of Theorem 8.5.3 by an application of Theorem 7.4.3 or Theorem 7.4.5. Therefore, we do not write out the proofs but only state the results.

The first result describes an algorithm for the construction of decompositions with respect to transductions for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ on classes of structures of bounded degree.

Theorem 8.5.5. *There is an algorithm which, on input of*

- *a degree bound $d \geq 2$,*
- *relational signatures σ and τ,*
- *an arity $s \geq 1$,*
- *a transduction Θ from σ_s to τ with arity $t \geq 1$ and quantifier rank $q_\Theta \geq 0$, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}[\tau]$ with $U \subseteq U_{\mathrm{all}}$, $n \coloneqq |\overline{x}|$ free variables, quantifier weight $w \geq 2$, and quantifier rank $q \geq 0$,*

computes a Θ-decomposition $\Delta = (\beta, \Delta_1, \ldots, \Delta_s)$ over $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)[\sigma]$ for $\varphi(\overline{x})$ on $\mathfrak{C}^{d,\sigma}$, where all the formulae in the sets $\Delta_1, \ldots, \Delta_s$ are HNF*-formulae with quantifier weight $< 2w + (t \cdot (n{+}q) + q_\Theta) \cdot \nu_d(4^{t \cdot q + q_\Theta})$.*

Furthermore, the algorithm computes Δ in time

$$||\Theta|| \cdot \mathcal{O}(||\tau||) + 2^{\left(||\Theta|| \cdot ||\varphi|| \cdot 2^{(t \cdot q + q_\Theta) \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}}.$$

and with size in

$$2^{\left(||\Theta|| \cdot ||\varphi|| \cdot 2^{(t \cdot q + q_\Theta) \cdot (\log w)^2} \cdot \nu_d(4^q)\right)^{\mathcal{O}(||\sigma_s||)}}.$$

The second result describes an algorithm for the construction of $\otimes$-decompositions for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ on classes of structures of bounded degree.

Theorem 8.5.6. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$*,*
- *a relational signature* σ*,*
- *an arity* $s \geq 1$*, and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}[\sigma_s]$ *with* $U \subseteq U_{\mathrm{all}}$*,* $n := |\overline{x}|$ *free variables, quantifier weight* $w \geq 2$*, and quantifier rank* $q \geq 0$*,*

computes an s*-ary* $\otimes$*-decomposition* $(\beta, \Delta_1, \ldots, \Delta_s)$ *for* $\varphi(\overline{x})$ *over* $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)[\sigma]$ *on* $\mathfrak{C}^{d,\sigma}$*, where all formulae in the sets* $\Delta_1, \ldots, \Delta_s$ *are* HNF*-formulae with threshold* $< 2w + s \cdot (n{+}q) \cdot \nu_d(4^{s \cdot q})$*.*

Furthermore, the algorithm computes Δ *in time*

$$2^{\left(||\varphi|| \cdot 2^{q \cdot (\log w)^2} \cdot \nu_d(4^{s \cdot q})\right)^{\mathcal{O}(||\sigma_s|| \cdot \log ||\sigma_s||)}}.$$

8.6 Preservation Theorems

In this section, we generalise the algorithms of Section 7.5 further to formulae from logics $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}$ with $U \subseteq U_{\mathrm{all}}$.

More precisely, we show how to construct existential formulae for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}$ that are preserved under extensions on a class of bounded degree structures that is closed under disjoint unions and induced substructures. For formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U)_{\mathrm{tpl}}$ that are preserved under homomorphisms on this class (provided that the class is decidable), we show how to construct existential-positive formulae.

8.6.1 Preservation under Extensions

In this section, we prove the following generalisation of Theorem 7.5.1:

Theorem 8.6.1. *There is an algorithm which, on input of*

- *a degree bound* $d \geq 2$*,*
- *a relational signature* σ*, and*
- *a formula* $\varphi(\overline{x})$ *from* $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}[\sigma]$*,*

constructs an existential formula $\psi(\overline{x})$ *from* $\mathsf{FO}[\sigma]$ *such that the following holds for any class* $\mathfrak{D}$ *of* d*-bounded* σ*-structures that is closed under disjoint unions* *and induced substructures: If $\varphi(\overline{x})$ is preserved under extensions on $\mathfrak{D}$, then $\varphi(\overline{x})$ and $\psi(\overline{x})$ are $\mathfrak{D}$-equivalent.*

Furthermore, the algorithm computes $\psi(\overline{x})$ in time

$$||\varphi|| \cdot \Big(2^{\nu_d(2^{\nu_d(4^q)^{\mathcal{O}(||\sigma||)}})} \cdot (w{+}n{+}q) \cdot L\Big)^{(n+q)\cdot\mathcal{O}((\log w)^2)}$$

where $w \geq 2$ and $n, q \geq 0$ are the quantifier weight, the number of free variables, and the quantifier rank of $\varphi(\overline{x})$, respectively, and where $L \geq 1$ is the least common multiple of the periods of all ultimately periodic counting quantifiers in $\varphi(\overline{x})$.

In particular, the constants suppressed by the $\mathcal{O}$-notation do not depend on the signature σ.

Remark 8.6.2. Under the assumption that $||\sigma|| < ||\varphi||$, and since $w, n, q < ||\varphi||$ and $L \leq 2^{||\varphi||^2}$, the algorithm of Theorem 8.6.1 takes 5-fold exponential time in the size of $\varphi(\overline{x})$ for degree bounds $d \geq 3$, and 3-fold exponential time for $d = 2$.

Proof. Let $d \geq 2$ be a degree bound, let σ be a relational signature, and let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}[\sigma]$ with quantifier weight $w \geq 2$, $n \geq 0$ free variables, quantifier rank $q \geq 0$. Let $U \subseteq U_{\mathrm{all}}$ be the set of all ultimately periodic counting quantifiers that occur in $\varphi(\overline{x})$, and let $L \geq 1$ be the least common multiple of the periods of the quantifiers in U.

The algorithm proceeds in the following two steps:

(Step 1) The algorithm of Lemma 8.3.1 constructs a formula $\tilde{\varphi}(\overline{x})$ from the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{M}(D^U)_{\mathrm{tpl}}[\sigma]$ that is equivalent to $\varphi(\overline{x})$, has the same quantifier rank as $\varphi(\overline{x})$, and threshold and maximum period $< w$. This takes time in

$$\mathcal{O}(||\varphi||) \cdot \mathcal{O}(w)^q. \tag{1}$$

Note that, in particular, L is also the least common multiple of the periods of all modulo-counting quantifiers in D^U.

(Step 2) The algorithm of Theorem 7.5.1 constructs, on input of d, σ, and $\tilde{\varphi}(\overline{x})$, an existential formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ such that for each class $\mathfrak{D}$ of d-bounded σ-structures that is closed under disjoint unions and induced substructures, if $\tilde{\varphi}(\overline{x})$ (respectively, $\varphi(\overline{x})$) is closed under extensions on $\mathfrak{D}$, then $\varphi(\overline{x})$ and $\psi(\overline{x})$ are $\mathfrak{D}$-equivalent. This takes time in

$$\begin{aligned} &\mathcal{O}(||\varphi||) \cdot \mathcal{O}(w)^q \cdot \Big(2^{\nu_d(2^{\nu_d(4^q)^{\mathcal{O}(||\sigma||)}})} \cdot (w{+}n{+}q) \cdot L\Big)^{(n+q)\cdot\mathcal{O}((\log w)^2)} \\ \subseteq\ & ||\varphi|| \cdot \Big(2^{\nu_d(2^{\nu_d(4^q)^{\mathcal{O}(||\sigma||)}})} \cdot (w{+}n{+}q) \cdot L\Big)^{(n+q)\cdot\mathcal{O}((\log w)^2)}. \end{aligned} \tag{2}$$

Adding up Estimate (1) and Estimate (2), we obtain that Estimate (2) is also an upper bound on the running time of the algorithm. This completes the proof of Theorem 8.6.1. □

8.6.2 Preservation under Homomorphisms

In this section, we show the following generalisation of Theorem 7.5.5. Its proof is particularly straightforward, since already the upper bounds on the size of minimal models for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ and $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ did not depend on the threshold or maximum period of the formulae, and since Lemma 6.3.2 for the construction of existential-positive formulae was already stated for arbitrary ultimately periodic logics.

Theorem 8.6.3. *Let $\mathfrak{C}'$ a class of structures that is decidable in time $t(n)$ for some function $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$ and that is closed under disjoint unions and induced substructures.*

There is an algorithm which, on input of

- *a degree bound $d \geq 2$,*
- *a relational signature σ, and*
- *a formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}[\sigma]$,*

constructs an existential-positive formula $\psi(\overline{x})$ from $\mathsf{FO}[\sigma]$ such that the following holds for the class $\mathfrak{D}$ of d-bounded σ-structures from $\mathfrak{C}'$: If $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, then $\varphi(\overline{x})$ and $\psi(\overline{x})$ are $\mathfrak{D}$-equivalent.

Furthermore, the algorithm computes $\psi(\overline{x})$ in time

$$2^{||\varphi||\cdot(n+1)^{\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}} \cdot t\big((n+1)^{\mathcal{O}(||\sigma||)} \cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}\big)$$

where $n, q \geq 0$ are the number of free variables and the quantifier rank of $\varphi(\overline{x})$, respectively, and the formula $\psi(\overline{x})$ is of size

$$2^{(n+1)^{||\varphi||\cdot\mathcal{O}(||\sigma||)}\cdot 2^{\nu_d(2\cdot 4^q)^{\mathcal{O}(||\sigma||)}}}.$$

Remark 8.6.4. Note that the upper bounds on the size of the computed existential-positive sentence and the time required for its construction are the same as in Theorem 8.6.3 and Theorem 6.1.10.

In particular, if $t\colon \mathbb{N}_{\geq 1} \to \mathbb{N}_{\geq 1}$ is at most 1-fold exponential and if we assume that σ only contains relation symbols that actually occur in the input formula $\varphi(\overline{x})$, then the algorithm of Theorem 8.6.3 takes 4-fold exponential time in the size of $\varphi(\overline{x})$ for degree bounds $d \geq 3$, and 3-fold exponential time for $d = 2$.

The proof of Theorem 8.6.3 has the same structure as the ones for Theorem 6.1.10 and Theorem 7.5.5. In the first step, we find upper bounds on the size of the minimal models of formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$. As already the corresponding upper bound for $\mathsf{FO}{+}\mathrm{un}\mathsf{M}$ and $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}$ only depends on the number of free variables and the quantifier rank of the formulae (apart from the degree bound and the signature), we get the same upper bound for $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$.

Corollary 8.6.5. *There is a function*

$$N^{d,\|\sigma\|}(n,q) \quad \in \quad (n{+}1) \cdot S^{d,\|\sigma\|}(2 \cdot 4^q)$$

such that the following holds for every relational signature σ, each degree bound $d \geq 2$, every class $\mathfrak{D}$ of d-bounded σ-structures that is closed under disjoint unions and induced substructures, and every formula $\varphi(\overline{x})$ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}[\sigma]$:

If $\varphi(\overline{x})$ is preserved under homomorphisms on $\mathfrak{D}$, then every $\mathfrak{D}$-minimal model of $\varphi(\overline{x})$ has a universe of size at most $N^{d,\|\sigma\|}(n,q)$, where $n, q \geq 0$ are the number of free variables and the quantifier rank of $\varphi(\overline{x})$, respectively.

Proof. Let σ be a relational signature, let $d \geq 2$ be a degree bound, and let $\mathfrak{D}$ be a class of d-bounded σ-structures that is closed under disjoint unions and induced substructures.

Let $\varphi(\overline{x})$ be a formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}[\sigma]$ with $n \geq 0$ free variables and quantifier rank $q \geq 0$. By Lemma 8.3.1 there is a formula $\tilde{\varphi}(\overline{x})$ in $\mathsf{FO}{+}\mathrm{un}\mathsf{M}_{\mathrm{tpl}}[\sigma]$ with the same number of free variables and the same quantifier rank as $\varphi(\overline{x})$ and that is equivalent to $\varphi(\overline{x})$.

Suppose that $\varphi(\overline{x})$ and $\tilde{\varphi}(\overline{x})$ are preserved under homomorphisms on $\mathfrak{D}$. By Corollary 7.5.7, every $\mathfrak{D}$-minimal model of $\tilde{\varphi}(\overline{x})$ has a universe of size at most $N^{d,\|\sigma\|}(n,q)$ for the function already provided by Theorem 6.3.1. This completes the proof of Corollary 8.6.5. ☐

With this, we are ready to prove Theorem 8.6.3.

Proof sketch of Theorem 8.6.3. The proof of Theorem 8.6.3 proceeds in exactly the same fashion and with the same estimates as the proof of Theorem 6.1.10 and Theorem 7.5.5. The only difference is the use of Corollary 8.6.5 instead of Theorem 6.3.1 and Corollary 7.5.7, respectively, for the upper bound on the size of minimal models. ☐

8.7 Conclusion

In this chapter, we have finally generalised our main algorithmic results of the previous chapters to all ultimately periodic logics.

Let us focus on the case of degree bounds $d \geq 3$. Concerning Hanf normal form, we have shown that for each formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$, a d-equivalent HNF-formula can be computed in 3-fold exponential time in the size of the input formula. This also led us to a locality theorem for $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ in the manner of Nurmonen's theorem [Nur00] and to a model-checking algorithm for formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ and d-bounded structures that requires linear time in the size of the input structure and 3-fold exponential time in the size of the input formulae.

Furthermore, we have shown that the logic $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ is also, in a sense, the largest logic for which HNF-formulae exist. More precisely, even for the simple sentence $\mathsf{S}y\,y{=}y$ where $\mathsf{S} \subseteq \mathbb{N}$ is *not* ultimately periodic, no d-equivalent HNF-formulae exists for any degree bound $d \geq 0$ over the signature (P).

Regarding Feferman-Vaught decompositions, we have shown that for each formula from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$, decompositions with respect to disjoint sums, transductions over disjoint sums, and direct products on classes of d-bounded σ-structures can be computed in 3-fold exponential time.

Similarly to the case of Hanf normal form, we have furthermore seen that formulae with quantifiers that are not ultimately periodic do not necessarily have decompositions with respect to disjoint sums.

Finally, we have extended our algorithms for the construction of existential (existential-positive) formulae to formulae from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ that are preserved under extensions (homomorphisms) on a class of d-bounded structures with certain closure properties. For preservation under extensions, our algorithm needs 5-fold exponential time in the size of the input formulae, and for preservation under homomorphisms, the algorithm requires 4-fold exponential time.

In the next chapter we will see that, in particular, our algorithms for Hanf normal form, Gaifman normal form, and decompositions with respect to disjoint sums have worst-case optimal time complexity. For our upper bounds concerning preservation under extensions and homomorphisms, we will provide 3-fold exponential lower bounds.

9 Lower Bounds

In this chapter, we provide lower bounds for the construction of Hanf normal form, Gaifman normal form, and Feferman-Vaught decompositions on classes of structures of bounded degree, showing that our respective algorithms presented in the previous chapters are basically worst-case optimal. The lower bound for Hanf normal form is based on [BK12], while the lower bounds for Gaifman normal form and Feferman-Vaught decompositions are based on [Hei12, HKS13] and [HHS14, HHS15], respectively.

For the construction of existential or existential-positive formulae for formulae that are preserved under extensions or homomorphisms on classes of structures of bounded degree we present 3-fold exponential lower bounds from [HHS14, HHS15].

9.1 Introduction

In the previous chapters, we have presented algorithms for the construction of various normal forms on classes of structures of bounded degree which, in particular, provided us with elementary upper bounds on the time required to compute these normal forms. The aim of this chapter is to find corresponding lower bounds.

For Hanf normal form, we have proven in Section 8.4 (see Remark 8.4.3) that, even for formulae φ from $\mathsf{FO}{+}\mathrm{unC}(U_{\mathrm{all}})_{\mathrm{tpl}}$, d-equivalent HNF-formulae can be computed in time

$$2^{2^{\mathrm{poly}(||\varphi||)}} \quad \text{for } d = 2, \text{ and in time} \quad 2^{d^{2^{\mathcal{O}(||\varphi||)}}} \quad \text{for } d \geq 3.$$

In Section 9.3, we show that this cannot be improved substantially. Even for sentences φ from FO, there are no algorithms for the construction of d-equivalent HNF-formulae that terminate in time

$$2^{2^{o(||\varphi||)}} \quad \text{for } d = 2, \text{ or in time} \quad 2^{d^{2^{o(||\varphi||)}}} \quad \text{for } d \geq 3.$$

This generalises the lower bound of [BK12] to degree bounds $d = 2$ and $d > 3$.

For the construction of d-equivalent GNF-sentences for formulae φ from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}$, the upper bounds in terms of the size of the input formula implied by our algorithm in Chapter 4 (see Remark 4.1.8) and the lower bounds presented in Section 9.4 below are the same as for Hanf normal form and show that also this algorithm is basically worst-case optimal. The lower bounds for Gaifman normal form on structures of bounded degree extend the proofs of [Hei12, HKS13] to degree bounds > 3. The combinatorial essence of the proofs is distilled in a game characterisation.

According to Section 8.5, the construction of $\oplus$-decompositions with arity $s \geq 1$ for formulae φ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ and with respect to classes of d-bounded structures can be performed in time

$$2^{2^{s\cdot \mathrm{poly}(||\varphi||)}} \quad \text{for } d = 2, \text{ and in time} \quad 2^{d^{s\cdot 2^{\mathcal{O}(||\varphi||)}}} \quad \text{for } d \geq 3.$$

In Section 9.5, we will show that even for the construction of $\oplus$-decompositions of arity 2 for FO-sentences, there are no algorithms that terminate in time

$$2^{2^{o(||\varphi||)}} \quad \text{for } d = 2, \text{ or in time} \quad 2^{d^{2^{o(||\varphi||)}}} \quad \text{for } d \geq 3.$$

This lower bound is based on [HHS14, HHS15] and here generalised to degree bounds > 3.

In Section 8.6, we have shown that for formulae φ from $\mathsf{FO}{+}\mathrm{un}\mathsf{C}(U_{\mathrm{all}})_{\mathrm{tpl}}$ that are preserved under extensions (homomorphisms) on a class $\mathfrak{C}$ of structures of bounded degree that is closed under disjoint unions and induced substructures (and, for preservation under homomorphisms, decidable in 1-fold exponential time), a $\mathfrak{C}$-equivalent existential (existential-positive) sentence can be computed in 5-fold (4-fold) exponential time in the size of φ. In Section 9.6, we prove 3-fold exponential lower bounds for both cases that already hold for FO-sentences (see [HHS14, HHS15]).

The basic approach to the lower bounds presented in this chapter will be to find slow-growing sequences of formulae over a suitable signature for which we can find lower bounds on the *size* of corresponding normal forms in respect to a class of structures of bounded degree.

The following lemma shows how this leads to lower bounds on the running time of algorithms constructing the respective normal form.

Lemma 9.1.1. *Let Σ be a countable alphabet and let $L \subseteq \Sigma^*$. For each word $w \in L$, let $L_w \subseteq \Sigma^*$ be non-empty. Suppose that there is a number $h_0 \in \mathbb{N}_{\geq 1}$, a* *sequence* $(w_h)_{h \geq h_0}$ *of words from* L*, a number* $c \in \mathbb{N}_{\geq 1}$*, and strictly increasing functions* $f, g\colon \mathbb{N}_{\geq h_0} \to \mathbb{N}_{\geq 1}$*, such that for each* $h \geq h_0$*,*

(1) $|w_h| \ \leq \ c \cdot g(h)$*, and*

(2) every $v \in L_{w_h}$ *has size* $|v| \geq f(g(h))$*.*

Then, there is no algorithm which computes, on input of a word $w \in L$*, in time* $f(o(|w|))$ *an element of* L_w*.*

Note that, in the lemma, we speak about the input and the desired output of algorithms in terms of sets of words over some alphabet. Although we will only use the lemma with (representations) of FO-sentences over some signature as the set L of inputs, the lemma is phrased in this general way so that it can be fitted to the various normal forms like Hanf normal form, Gaifman normal form, and $\oplus$-decompositions we wish to compute.

Proof of Lemma 9.1.1. Let Σ be a countable alphabet and let $L \subseteq \Sigma^*$. For each $w \in L$, let $L_w \subseteq \Sigma^*$ be a non-empty set. Let $h \in \mathbb{N}_{\geq 1}$, let $(w_h)_{h \geq h_0}$ be a sequence of words from L, let $c \in \mathbb{N}_{\geq 1}$, and let $f, g\colon \mathbb{N}_{\geq h_0} \to \mathbb{N}_{\geq 1}$ be strictly increasing such that for all $h \geq h_0$, $|w_h| \leq c \cdot g(h)$ and every $v \in L_{w_h}$ has size $|v| \geq f(g(h))$.

Towards a contradiction, assume that there is a function $t(n) \in o(n)$ and an algorithm, which on input of a word $w \in L$, computes a word $v \in L_w$ in time $f(t(|w|))$. Then, in particular, $|v| \leq f(t(|w|))$.

For each $h \geq h_0$, the word v_h, computed by the algorithm on input of w_h, has size

$$f(g(h)) \quad \leq \quad |v_h| \quad \leq \quad f(t(|w_h|)) \quad \leq \quad f(t(c \cdot g(h))).$$

Hence, we have

$$g(h) \ \leq \ t(c \cdot g(h)) \quad \text{for each } h \geq h_0. \tag{1}$$

Consider the function $T(n) \coloneqq \frac{n}{t(n)}$. Since $t(n) \in o(n)$, there is an $H_0 \geq h_0$ such that $T(c \cdot g(h)) > c$ for all $h \geq H_0$. Therefore, for each $h \geq H_0$, we obtain

$$t(c \cdot g(h)) \quad = \quad \frac{c \cdot g(h)}{T(c \cdot g(h))} \quad < \quad g(h) \quad \leq \quad t(c \cdot g(h)). \tag{2}$$

With this contradiction, the proof of Lemma 9.1.1 is complete. $\square$

A key ingredient to obtain “small” sentences with “large” normal forms will be encodings of large initial segments of the natural numbers by trees of bounded degree that can be compared by small FO-formulae. We will introduce these tree encodings and some basic notation about trees in the subsequent Section 9.2.

Note that similar methods as used here go back to [SM73] and were also applied in [FG04, PV06] for lower bounds in parameterised complexity theory, and in [GS04, GS05] for lower bounds on the succinctness of logics. Furthermore, [DGKS07] obtained non-elementary lower bounds on the size of Gaifman normal form, Feferman-Vaught decompositions, and existential sentences on acyclic structures of arbitrary degree.

9.2 Tree Encodings

In this section, we introduce encodings of initial segments of the natural numbers by tree-like structures over various signatures. We will also show that "large" numbers in these encodings can be compared by "small" FO-formulae over the respective signature. This section can be optionally skipped and read later, when a specific encoding is used for the statement and proof of the lower bounds in the subsequent sections.

Trees and Forests

We commence with some general notation about *directed* trees. Recall that E is a binary relation symbol. A *tree* is a finite (E)-structure $\mathcal{T}$ which contains a node $a \in T$ such that for every node $b \in T$ there is precisely one path from a to b in $\mathcal{T}$. The node a is also called the *root* of $\mathcal{T}$.

A *forest* $\mathcal{F}$ is a finite disjoint union of trees. The *height of a node* $b \in F$ is the length of the unique path from the root node of its connected component to b, and the *height of the forest* $\mathcal{F}$ is the maximum height of all its nodes. The *parent* of a non-root node $b \in F$ is the unique node $c \in F$ such that $(c, b) \in E^{\mathcal{F}}$. A node $c \in F$ is a *successor (or, child)* of b if $(b, c) \in E^{\mathcal{F}}$. A *leaf* is a node that does not has any successors.

For each node $a \in F$ and every $\ell \geq 0$, the set $S_\ell^{\mathcal{F}}(a)$ denotes the set of all nodes in F that can be reached from a by a directed path of length at most ℓ, and $\mathcal{S}_\ell^{\mathcal{F}}(a)$ denotes the subtree of $\mathcal{F}$ with root a induced by the set $S_\ell^{\mathcal{F}}(a)$.[1]

[1]Note that this is similar to the notion of ℓ-neighbourhoods $N_\ell^{\mathcal{F}}(a)$ and ℓ-spheres $\mathcal{N}_\ell^{\mathcal{F}}(a)$, which, however, are defined by the distance measure provided by the Gaifman graph, and not by the length of directed paths in the forest.

Similarly, $S^{\mathcal{F}}(a)$ is the union of $S^{\mathcal{F}}_{\ell}(a)$ for all $\ell \geq 0$, and $\mathcal{S}^{\mathcal{F}}(a)$ is the subtree of $\mathcal{F}$ with root a induced by the set $S^{\mathcal{F}}(a)$.

By $\mathfrak{T}$ we denote the class of all trees, and by $\mathfrak{F}$ the class of all forests.

Tree-like and Forest-like Structures

In the following, we extend the notation just introduced to structures over signatures σ that, in a sense, look like forests. In particular, the Gaifman graph of such structures is the same as the Gaifman graph of a forest. Mostly, we will use this generalisation to talk about labelled and ordered forests.

Consider a signature σ that only contains binary relation symbols $S_0, \dots, S_n$ for some $n \geq 1$ and possibly further unary relation symbols. We call a σ-structure $\mathcal{A}$ *forest-like*, if the following conditions hold:

- The relations $S_0^{\mathcal{A}}, \dots, S_n^{\mathcal{A}}$ are pairwise disjoint and for each $a \in A$ and every $i \in [0, n]$, there is at most one $b \in A$ such that $(a, b) \in S_i^{\mathcal{A}}$.
- The structure $\mathcal{F}$ over the signature (E) with the same universe A, and where $E^{\mathcal{F}}$ is the disjoint union of the relations $S_0^{\mathcal{A}}, \dots, S_n^{\mathcal{A}}$, is a forest.

In particular, if $\mathcal{F}$ is a tree, then $\mathcal{A}$ is called *tree-like*. In a forest-like structure $\mathcal{A}$, the leaves of $\mathcal{A}$ are the leafs of $\mathcal{F}$, the height of a node from A is the height of the same node in $\mathcal{F}$, and the height of $\mathcal{A}$ is the height of $\mathcal{F}$. In the same way, we generalise the notions of parents and successors of nodes, and of reachable node sets and induced subtrees. Moreover, if $\mathcal{A}$ is tree-like, then the root of $\mathcal{F}$ is also the root of $\mathcal{A}$.

Sometimes we will also call forest-like and tree-like structures forests and trees, respectively, if this does not lead to ambiguity.

9.2.1 Labelled and Ordered Trees of Bounded Arity

In the following, we let L denote a unary relation symbol and we let $S_0, S_1, \dots$ denote binary relation symbols. Using these relation symbols we define, for each $d \geq 2$, a signature $\tau_d \coloneqq (L, S_0, \dots, S_{d-2})$.[2]

Let $d \geq 2$. A *labelled and ordered tree* $\mathcal{T}$ *of arity* $d-1$ is a tree-like structure over the signature τ_d where the binary relation symbols $S_0, \dots, S_{d-2}$ are interpreted as the j-th successor for $j \in [0, d-2]$, respectively. In particular, this means that

[2]Note that is not the same as the signatures $\sigma_s = (\sigma, P_1, \dots, P_s)$ for relational signatures σ and $s \geq 1$ used in Chapter 5.

for each node $a \in T$ and every $j \in [0, d{-}2]$, there is at most one j-th successor, that is, at most one node $b \in T$ with $(a, b) \in S_j^{\mathcal{T}}$. Clearly, $\mathcal{T}$ has degree $\leq d$.

By $\mathfrak{T}_d$ we denote the *class of all labelled and ordered trees of arity $d-1$*, and by $\mathfrak{F}_d$ the *class of all finite disjoint unions of labelled and ordered trees of arity $d-1$*.

We call a node $a \in T$ *full* if it has an S_j-successor for each $j \in [0, d{-}2]$. Furthermore, $\mathcal{T}$ is said to be *complete with height $\ell \geq 0$* if each of its nodes is either full or a leaf, and all leaves have height ℓ. For each $\ell \geq 0$, we let $\mathfrak{T}_{d,\ell}$ denote the *set of all (up to isomorphism) labelled and ordered trees of arity $d-1$ that are complete with height ℓ*.

Note that we can understand the structures in a set $\mathfrak{T}_{d,\ell}$ as encodings of natural numbers whose binary expansion is given by the labelling of the nodes of the structures. However, we will not speak about these numbers explicitly but just use that the structures in $\mathfrak{T}_{d,\ell}$ can be discriminated by small formulae. In particular for the case of $d = 3$, the corresponding labelled and ordered binary trees were also used in, e.g., [FG04, BK12] for proofs of lower bounds.

Observe that the structures in $\mathfrak{T}_{2,\ell}$, for each $\ell \geq 1$, are labelled paths of length ℓ and thus, each have $\ell + 1$ nodes. On the other hand, for degree bounds $d \geq 3$ and $\ell \geq 1$, any structure in $\mathfrak{T}_{d,\ell}$ has

$$\sum_{i=0}^{\ell}(d{-}1)^i \;=\; \frac{(d{-}1)^{\ell+1}-1}{d-2} \;>\; (d{-}1)^{\ell} \;\geq\; d^{\frac{\ell}{2}}$$

nodes. The latter inequality holds since $(d-1)^2 \geq d$ for all $d \geq 3$. This leads us to the following observation.

Observation 9.2.1. *There are function $f_d \colon \mathbb{N} \to \mathbb{N}_{\geq 1}$ with $d \geq 2$, for each $h \geq 0$ defined by*

$$f_2(h) \;:=\; 2^{2^h} \quad \text{if } d = 2, \qquad \text{and} \quad f_d(h) \;:=\; 2^{d^{2^{h-1}}} \quad \text{if } d \geq 3,$$

such that for each $d \geq 2$ and every $h \geq 0$,

$$|\mathfrak{T}_{d,2^h}| \;>\; f_d(h).$$

Observation 9.2.1 leads to the following corollary to Lemma 9.1.1, which we will use frequently in the subsequent sections of this chapter.

Corollary 9.2.2. *Let $d \geq 2$, let Σ be a countable alphabet, and let $L \subseteq \Sigma^*$. For each word $w \in L$, let $L_w \subseteq \Sigma^*$ be non-empty. Suppose that there is a sequence $(w_h)_{h\geq 1}$ of words from L and a number $c \in \mathbb{N}_{\geq 1}$, such that for each $h \geq 1$,* *(1)* $|w_h| \le c \cdot h$*, and*

(2) every $v \in L_{w_h}$ *has size* $|v| \ge |\mathfrak{T}_{d,2^h}|$*.*

Then, there is no algorithm which computes, on input of a $w \in L$*, in time*

$$2^{2^{o(|w|)}} \quad \textit{if } d = 2, \qquad \textit{and in time} \quad 2^{d^{2^{o(|w|)}}} \quad \textit{if } d \ge 3,$$

an element of L_w*.*

Proof. Let $d \ge 2$, let Σ be a countable alphabet, and let $L \subseteq \Sigma^*$. For each $w \in L$, let $L_w \subseteq \Sigma^*$ be a non-empty set. Suppose that there is a sequence $(w_h)_{h \ge 1}$ of words from L and a number $c \in \mathbb{N}_{\ge 1}$ such that for each $h \ge 1$, $|w_h| \le c \cdot h$ and every $v \in L_{w_h}$ has size $|v| \ge |\mathfrak{T}_{d,2^h}| \ge f_d(h)$, where $f_d \colon \mathbb{N} \to \mathbb{N}_{\ge 1}$ is the function defined in Observation 9.2.1.

For applying Lemma 9.1.1, we let $h_0 = 1$, $f \coloneqq f_d$ and g the identity function. With this, it follows, that there is no algorithm which computes, on input of a word $w \in L$, in time

$$2^{2^{o(|w|)}} \;=\; f_2(o(|w|))$$

a word $v \in L_w$.

For $d \ge 3$, Lemma 9.1.1 shows that there is no algorithm which computes, on input of a word $w \in L$, in time

$$2^{d^{2^{o(|w|)}}} \;\subseteq\; 2^{d^{2^{o(|w|)-1}}} \;=\; f_d(o(|w|))$$

a word $v \in L_w$.

This completes the proof of Corollary 9.2.2. $\square$

The formulae provided by the following lemma, which generalises [FG04, Lemma 25], show that the structures from the sets $\mathfrak{T}_{d,2^h}$ for $d \ge 2$ and $h \ge 1$ can be compared and recognised by comparatively "small" formulae. This will be crucial for the application of Corollary 9.2.2 in our proofs of lower bounds for structures of bounded degree.

Lemma 9.2.3 (cf. [FG04, Lemma 25])**.** *For each* $d \ge 2$*, there is a number* $c_d \in \mathbb{N}_{\ge 1}$ *and sequences* $(\mathrm{iso}_{d,h}(x, x'))_{h \ge 1}$ *and* $(\mathrm{complete}_{d,h}(x))_{h \ge 1}$ *of* $\mathsf{FO}[\tau_d]$*-formulae of size* $\le c_d \cdot h$*, such that for each* $h \ge 1$*, the following holds:*

(a) For each $\mathcal{F} \in \mathfrak{F}_d$ *and all* $a, a' \in F$ *where* $\mathcal{S}^{\mathcal{F}}_{2^h}(a)$ *and* $\mathcal{S}^{\mathcal{F}}_{2^h}(a')$ *are complete with height* 2^h*,*

$$\mathcal{F} \;\models\; \mathrm{iso}_{d,h}[a, a'] \quad \textit{iff} \quad \mathcal{S}^{\mathcal{F}}_{2^h}(a) \;\cong\; \mathcal{S}^{\mathcal{F}}_{2^h}(a').$$

(b) For each $\mathcal{F} \in \mathfrak{F}_d$ and all $a \in A$,

$$\mathcal{F} \models \text{complete}_{d,h}[a] \quad \textit{iff} \quad \mathcal{S}^{\mathcal{F}}(a) \textit{ is complete with height } 2^h.$$

For the proof of Lemma 9.2.3, some notation will be convenient. Let $d \geq 2$ and let $\ell \geq 0$. Consider a structure $\mathcal{F} \in \mathfrak{F}_d$, and let $a, b, a', b' \in F$. We call b, b' *co-reachable with distance* $\leq \ell$ from a, a' if and only if the following holds: There is a number $n \leq \ell$ and sequences $a = c_0, \ldots, c_n = b$ and $a' = c'_0, \ldots, c'_n = b'$ of nodes of $\mathcal{F}$ such that for every $i \in [0, n)$, there is a $j \in [0, d-2]$ such that (c_i, c_{i+1}) and (c'_i, c'_{i+1}) belong to the j-th successor relation $S_j^{\mathcal{F}}$. Intuitively, this means that b and b' can be reached from a and a', respectively, by paths using the same successor relations in the same order.

Proof of Lemma 9.2.3. Let $d \geq 2$. Before constructing the formulae $\text{iso}_{d,h}(x, x')$ and $\text{complete}_{d,h}(x)$ for $h \geq 1$, we define formulae that recognise co-reachable pairs of nodes up to a certain distance, and which only grow logarithmically with this distance.

Claim 1. *For each $\ell \geq 0$, there is an $\mathsf{FO}[\tau_d]$-formula $\text{co-reach}_{d,\ell}(x, y, x', y')$ such that for every $\mathcal{F} \in \mathfrak{F}_d$ and all $a, b, a', b' \in F$,*

$$\mathcal{F} \models \text{co-reach}_{d,\ell}[a, b, a', b']$$

iff $\quad$ *b, b' are co-reachable from a, a' with distance $\leq \ell$.*

Proof of Claim 1. We construct the formulae by an induction on $\ell \geq 0$, following Lemma 25 in [FG04]. For $\ell = 0$, we let

$$\text{co-reach}_{d,0}(x, y, x', y') \ :=\ x{=}y \ \wedge \ x'{=}y',$$

and for $\ell = 1$, we let

$$\begin{aligned}\text{co-reach}_{d,1}(x, y, x', y') \ :=\ & \text{co-reach}_{d,0}(x, y, x', y') \\ & \vee \bigvee_{j=0}^{d-2} \left(S_j(x, y) \ \wedge \ S_j(x', y')\right).\end{aligned}$$

For all $\ell \geq 1$, we let

$$\begin{aligned}\text{co-reach}_{d,2\ell}(x, y, x', y') \ :=\ \exists z \exists z' \forall u \forall v \forall u' \forall v' \Big(& ((u{=}x \wedge u'{=}x' \wedge v{=}z \wedge v'{=}z') \vee \\ & (u{=}z \wedge u'{=}z' \wedge v{=}y \wedge v'{=}y')) \\ & \to \ \text{co-reach}_{d,\ell}(u, v, u', v')\Big)\end{aligned}$$

and

$$\text{co-reach}_{d,2\ell+1}(x,y,x',y') \;:=\; \exists z \exists z' \,(\text{co-reach}_{d,1}(x,z,x',z') \\ \wedge\; \text{co-reach}_{d,2\ell}(z,y,z',y')).$$

After proving Claim 1, we now turn to the construction of the formulae $\text{iso}_{d,h}(x,x')$ and $\text{complete}_{d,h}(x)$. Let $h \geq 1$.

(a) The formula

$$\text{iso}_{d,h}(x,x') \;:=\; \forall y \forall y' \Big(\text{co-reach}_{d,2^h}(x,y,x',y') \;\rightarrow\; (L(y) \leftrightarrow L(y'))\Big)$$

states that, up to distance 2^h, each two nodes y and y' that are in the same position in the tree below x and x', respectively, are labelled in the same way. This suffices, since we suppose that the subtrees below x and x' are complete with height 2^h.

(b) For each $\ell \geq 0$, we let

$$\text{reach}_{d,\ell}(x,y) \;:=\; \text{co-reach}_{d,\ell}(x,y,x,y),$$

which is satisfied if there is any path of length $\leq \ell$ from x to y. With this, we let

$$\begin{aligned}\text{complete}_{d,h}(x) \;:=\;\; & \exists y \Big(\text{reach}_{d,2^h}(x,y) \;\wedge\; \neg\,\text{reach}_{d,2^h-1}(x,y)\Big) \\ & \wedge\; \forall y \Big(\big(\text{reach}_{d,2^h}(x,y) \wedge \neg\,\text{reach}_{d,2^h-1}(x,y)\big) \\ & \qquad \rightarrow\; \neg \bigvee_{j=0}^{d-2} \exists z\, S_j(y,z)\Big) \\ & \wedge\; \forall y \Big(\text{reach}_{d,2^h-1}(x,y) \;\rightarrow \bigwedge_{j=0}^{d-2} \exists z\, S_j(y,z)\Big).\end{aligned}$$

Here, the first, second, and third line together state that the subtree below x has height precisely 2^h, and the fourth line states that every node of height less than 2^{h-1} is full.

By induction on the inductive definition of the formulae $\text{co-reach}_{d,\ell}(x,y,x',y')$ it can be shown straightforwardly that there is a number $c_d \in \mathbb{N}_{\geq 1}$ such that for all $h \geq 1$, the formulae $\text{iso}_{d,h}(x,x')$ and $\text{complete}_{d,h}(x)$ have size $\leq c_d \cdot h$. This completes the proof of Lemma 9.2.3. $\square$

In the next section, we introduce some notation about the special case of labelled and ordered trees with arity 1, which we call labelled chains.

9.2.2 Labelled Chains

Sometimes, we also call the ordered and labelled unary trees from the class $\mathfrak{T}_2$ *labelled chains*, and mean by the *length* of a labelled chain its height.

A labelled chain of length $\ell \geq 0$ can be represented by a bit string, that is, a word $w = w_0, \ldots, w_\ell$ over the alphabet $\{0, 1\}$ of length $\ell + 1$. In particular, we denote by $\mathcal{C}_w$ the labelled chain with universe $a_0, \ldots, a_\ell$, where, for all $i, j \in [0, \ell)$, $a_i \in L^{\mathcal{C}_w}$ if and only if $w_i = 1$, and where $(a_i, a_j) \in S_0^{\mathcal{C}_w}$ if and only if $j = i + 1$. We also say that a node a of a labelled chain $\mathcal{C}$ is labelled with 0 if $a \in L^{\mathcal{C}}$, and labelled with 1 otherwise.

9.2.3 Unordered Trees

This section provides encodings of natural numbers by unordered trees, that is, trees over the signature (E). First, we recall an encoding of numbers by unordered trees of arbitrarily high degree from [FG06, Chapter 10] (see also [DGKS07]). For a parameter $h \geq 0$, this encoding allows to compare numbers from an initial segment of size $\mathrm{Tower}(h)$ of the natural numbers by formulae of size linear in h. Recall that $\mathrm{Tower}(0) = 1$ and, for each $h \geq 1$,

$$\mathrm{Tower}(h) \quad = \quad 2^{2^{\cdot^{\cdot^{\cdot^{2}}}}} \Big\} \text{ a tower of } 2s \text{ of height } h.$$

Afterwards, we will adapt this encoding to an encoding of numbers by binary trees (cf., [Hei12, HKS13]). For each $h \geq 0$, this encoding allows to express arithmetics over an initial segment of size $\mathrm{Tower}(h{+}3)$ of the natural numbers by formulae of size linear in $\mathrm{Tower}(h)$.

One advantage of the encoding of numbers by (binary) trees is that they do not require the edges of the trees to be ordered, and they also do not require a labelling of the trees. However, the main advantage is that they not only allow to compare numbers encoded as trees by short formulae, but also to express arithmetics over these numbers. We will make use of this in Section 9.6.

Trees of Arbitrary Degree

In this section, we recall the definition of the tree encoding from [FG06, DGKS07], and cite a lemma that provides us with "small" formulae to compare such tree encodings.

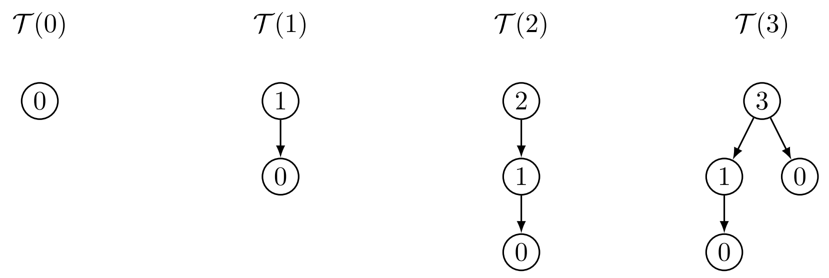

Figure 9.1 Tree encodings for the numbers 0, 1, 2, and 3. Note that the numbers depicted within the nodes are *not* part of the tree encoding; they are just indicated here to illustrate which number is encoded by the subtree starting at the respective node.

Definition 9.2.4. Let $i \in \mathbb{N}$. The *tree encoding* $\mathcal{T}(i)$ of i is a tree over the signature (E), defined inductively as follows:

- $\mathcal{T}(0)$ is the one-node tree.
- For $i \geq 1$, the tree $\mathcal{T}(i)$ is obtained by creating a new root and attaching to it all trees $\mathcal{T}(j)$ for all $j \in \mathbb{N}$ such that $\mathrm{bit}(j, i) = 1$.

(See Figure 9.1 and Figure 9.2(b) for illustrations.)

Remark 9.2.5. By induction it can easily be shown that for each $h \geq 0$, all tree encodings $\mathcal{T}(i)$ with $i < \mathrm{Tower}(h)$ have height $\leq h$.

The following lemma from [FG06, DGKS07] shows that tree encodings of numbers can be compared by "small" $\mathsf{FO}[E]$-formulae.

Lemma 9.2.6 ([FG06, Lemma 10.21]). *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\mathrm{eq}'_h(x, y))_{h \geq 0}$ of $\mathsf{FO}[E]$-formulae of size $\leq c \cdot h$, for each $h \geq 1$, such that for each $h \geq 0$, every forest $\mathcal{F} \in \mathfrak{F}$, and all nodes $a, b \in F$, the following holds:*

If there are $i, j \in [0, \mathrm{Tower}(h))$ such that $\mathcal{S}^{\mathcal{F}}(a) \cong \mathcal{T}(i)$ and $\mathcal{S}^{\mathcal{F}}(b) \cong \mathcal{T}(j)$, then

$$\mathcal{F} \models \mathrm{eq}'_h[a, b] \quad \textit{iff} \quad i = j.$$

We do not prove the latter here. However, the idea of the construction of the formulae is contained in Lemma 9.2.8 in the following section.

Binary Trees

The starting point for the encoding of numbers by binary trees, introduced in this section, is the encoding of numbers by trees (of arbitrary degree) that we just have recapitulated. The basic idea is to replace nodes with > 2 children by complete binary trees of sufficient height to whose leaves these children are then connected.

In the following, we denote by $\mathfrak{BF}$ and $\mathfrak{BT}$ the class of all *binary forests*, that is, 3-bounded forests from $\mathfrak{F}$ and the class of all *binary trees*, that is, 3-bounded trees from $\mathfrak{T}$, respectively. We call a binary tree $\mathcal{B}$ *complete with height* $\ell \geq 0$, if all leaves of $\mathcal{B}$ have height ℓ and every non-leaf node has exactly two children.

Definition 9.2.7. For each $h \geq -1$ and every number $i \in [0, \text{Tower}(h{+}3))$, we define inductively a set $\mathfrak{B}_h(i)$ of binary trees that (each) encode the (binary expansion of the) number i.

($h = -1$) For each $i \in [0, \text{Tower}(2)) = \{0, 1, 2, 3\}$, the set $\mathfrak{B}_{-1}(i)$ contains exactly the (binary trees) that are isomorphic to the tree encoding $\mathcal{T}(i)$ depicted in Figure 9.1.

($h \geq 0$) For each $i \in [0, \text{Tower}(h{+}3))$, the set $\mathfrak{B}_h(i)$ consists of all binary trees $\mathcal{B}$ with root $a \in B$ that satisfy each of the following properties:

- The induced subtree $\mathcal{S}^{\mathcal{B}}_{\text{Tower}(h+1)-1}(a)$ is complete with height $\text{Tower}(h{+}1) - 1$.
- For every $j \in [0, \text{Tower}(h{+}2))$ with $\text{bit}(j, i) = 1$, there is a node b of height $\text{Tower}(h{+}1)$ in $\mathcal{B}$ such that $\mathcal{S}^{\mathcal{B}}(b) \in \mathfrak{B}_{h-1}(j)$.
- For every node b of height $\text{Tower}(h{+}1)$ in $\mathcal{B}$, there is a number $j \in [0, \text{Tower}(h{+}2))$ such that $\mathcal{S}^{\mathcal{B}}(b) \in \mathfrak{B}_{h-1}(j)$ and $\text{bit}(j, i) = 1$.

Each tree in $\mathfrak{B}_h(i)$ is called a *binary tree encoding of i with parameter h*.

An example of a binary tree encoding of $i = 42$ with parameter $h = 1$ is depicted in Figure 9.2(b) (in comparison to the corresponding tree encoding of 42, which is *not* a binary tree). An induction on the parameter h shows that every number $i \in [0, \text{Tower}(h{+}3))$ has at least one binary tree encoding with parameter h.

An adaptation of Lemma 9.2.6 shows that there are $\mathsf{FO}[E]$-formulae that can compare binary tree encodings of “3-fold exponentially larger” numbers.

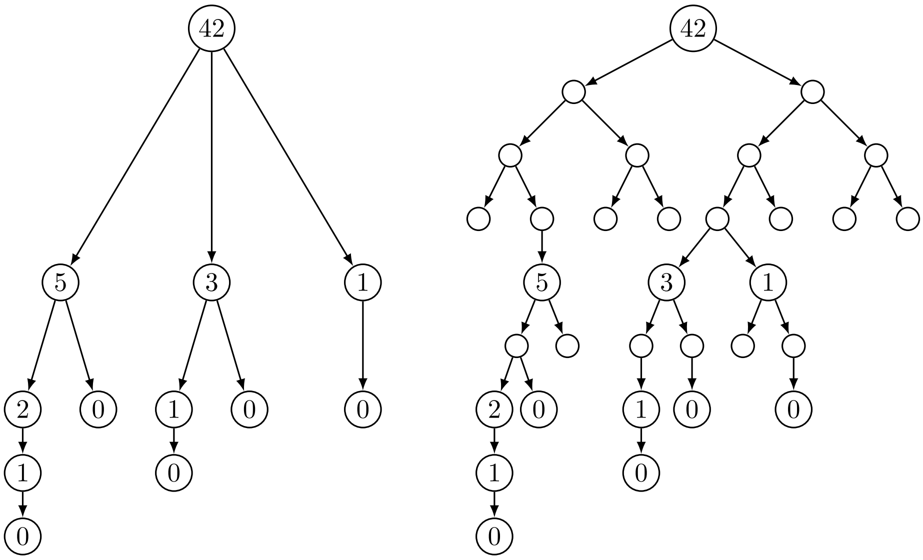

Figure 9.2 The figure to the left shows the tree encoding $\mathcal{T}(42)$ of the number 42. On the right, a binary tree encoding with parameter 1 of the number 42, that is, an element of the set $\mathfrak{B}_1(42)$, is depicted. Note that the numbers depicted within some of the nodes are *not* part of the encoding, they are just indicated here to illustrate which number is encoded by the subtree starting at the respective node.

Lemma 9.2.8. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\mathrm{eq}_h(x,y))_{h \geq -1}$ of $\mathsf{FO}[E]$-formulae of size $\leq c \cdot \mathrm{Tower}(h)$, for $h \geq 0$, such that for each $h \geq 0$, every $\mathcal{F} \in \mathfrak{B}\mathfrak{F}$, and all nodes $a, b \in F$, the following holds:*

If there are numbers $i, j \in [0, \mathrm{Tower}(h{+}3))$ such that $\mathcal{S}^{\mathcal{F}}(a) \in \mathfrak{B}_h(i)$ and $\mathcal{S}^{\mathcal{F}}(b) \in \mathfrak{B}_h(j)$, then

$$\mathcal{F} \models \mathrm{eq}_h[a,b] \quad \textit{iff} \quad i = j.$$

A straightforward induction shows the following observation, which will turn out useful for finding the upper bound on the size of the formulae of Lemma 9.2.8.

Observation 9.2.9. *For all $h \geq 0$,*

$$\sum_{i=0}^{h} \mathrm{Tower}(i) \;<\; 2 \cdot \mathrm{Tower}(h).$$

Proof of Lemma 9.2.8. *For $h = -1$*, a formula $\mathrm{eq}_{-1}(x,y)$ that is satisfied by two nodes a, b in a binary forest $\mathcal{F}$, if and only if $\mathcal{S}^{\mathcal{F}}(a)$ and $\mathcal{S}^{\mathcal{F}}(b)$ are isomorphic to the same tree $\mathcal{T}(i)$ for an $i \in \{0,1,2,3\}$ can be straightforwardly defined.

For $h \geq 0$, the construction of the formula $\mathrm{eq}_h(x,y)$ is best understood by keeping the binary expansions of the numbers encoded by binary trees in mind. That is, the formula expresses that every bit set in the binary expansion of the number i encoded by the subtree below x, the same bit is also set in the binary expansion of the number j encoded by the subtree below y, and vice versa.

To traverse the complete binary trees connecting the root node with the nodes representing the bits of the binary expansion of the encoded numbers, recall the formulae provided by Lemma 2.7.1. There is a sequence of $\mathsf{FO}[E]$-formulae $(\mathrm{path}_{\leq n}(x,y))_{n \geq 1}$ of size $\mathcal{O}(\log n)$, such that for each graph $\mathcal{A}$ and all $a, b \in A$,

$$\mathcal{A} \models \mathrm{path}_{\leq n}[a,b] \quad \text{iff} \quad \text{there is a path of length} \leq n \text{ from } a \text{ to } b \text{ in } \mathcal{A}.$$

In the following, we let

$$\pi_h(x,y) \;:=\; \mathrm{path}_{\leq \mathrm{Tower}(h+1)}(x,y) \;\wedge\; \neg\, \mathrm{path}_{\leq \mathrm{Tower}(h+1)-1}(x,y)$$

be the formula expressing that there is a path of length *precisely* Tower(h+1) between x and y. Clearly, $\pi_h(x,y)$ is of size $\mathcal{O}(\mathrm{Tower}(h))$. With this, we let

$$\begin{aligned}
\mathrm{eq}_h(x,y) \;\coloneqq\; & \Big(\exists x'\pi_h(x,x') \;\leftrightarrow\; \exists y'\pi_h(y,y')\Big) \wedge \\
& \forall x'\Big(\pi_h(x,x') \;\rightarrow \\
& \quad \exists y'\Big(\pi_h(y,y') \;\wedge \\
& \qquad \forall y''(\pi_h(y,y'') \;\rightarrow \\
& \qquad\quad \exists x''(\pi_h(x,x'') \;\wedge \\
& \qquad\qquad \forall u \forall v(((u{=}x' \wedge v{=}y') \vee (u{=}x'' \wedge v{=}y'')) \\
& \qquad\qquad\qquad \rightarrow\; \mathrm{eq}_{h-1}(u,v)))))\Big)\Big)
\end{aligned}$$

For the size of $\mathrm{eq}_h(x,y)$, it follows from Observation 9.2.9 that there is a number $c \in \mathbb{N}_{\geq 1}$ such that $||\,\mathrm{eq}_h\,|| \leq c \cdot \mathrm{Tower}(h)$ for all $h \geq 0$. This completes the proof of Lemma 9.2.8. ☐

In the following sections, the latter construction is used together with the following corollary to Lemma 9.1.1 for lower bounds on the complexity of constructing normal forms on the class $\mathfrak{BF}$.

Corollary 9.2.10. *Let Σ be a countable alphabet and $L \subseteq \Sigma^*$. For each word $w \in L$, let $L_w \subseteq \Sigma^*$ be non-empty. Suppose that there is a number $h_0 \in \mathbb{N}_{\geq 1}$, a sequence $(w_h)_{h \geq h_0}$ of words from L, and a number $c \in \mathbb{N}_{\geq 1}$, such that for each $h \geq h_0$:*

(1) $|w_h| \leq c \cdot \mathrm{Tower}(h)$*, and*

(2) every $v \in L_{w_h}$ *has size* $|v| \geq \mathrm{Tower}(h{+}3)$.

Then, there is no algorithm which computes, on input of a word $w \in L$, in time

$$2^{2^{2^{o(|w|)}}}$$

an element of L_w.

Proof. Let Σ be a countable alphabet and let $L \subseteq \Sigma^*$. For each word $w \in L$, let $L_w \subseteq \Sigma^*$ be a non-empty set. Suppose that there is a number $h_0 \in \mathbb{N}_{\geq 1}$, a sequence $(w_h)_{h \geq 1}$ of words from L and a number $c \in \mathbb{N}_{\geq 1}$, such that for each $h \geq h_0$, $|w_h| \leq c \cdot \mathrm{Tower}(h)$ and every $v \in L_{w_h}$ has size

$$|v| \;\geq\; \mathrm{Tower}(h{+}3) \;=\; 2^{2^{2^{\mathrm{Tower}(h)}}}$$

For an application of Lemma 9.1.1, we let $f, g\colon \mathbb{N}_{\geq h_0} \to \mathbb{N}_{\geq 1}$ be defined such that $f(h) := 2^{2^{2^h}}$ and $g(h) := \mathrm{Tower}(h)$ for each $h \geq h_0$. Then, it follows that there is no algorithm which computes, on input of a word $w \in L$, in time

$$2^{2^{2^{o(|w|)}}} \;=\; f(o(|w|))$$

a word $v \in L_w$. This completes the proof of Corollary 9.2.10. □

9.3 Hanf Normal Form

In this section, we show that the algorithm of Theorem 3.2.1 and thus also the algorithms of Theorem 7.3.1 and Theorem 8.4.2 for the construction of Hanf normal are basically worst-case optimal. The lower bounds already hold for the special case of input formulae from FO. For every degree bound $d \geq 2$, recall that $\mathfrak{F}_d$ is the class of labelled and ordered forests of arity $d-1$ over the signature τ_d, defined in Section 9.2.1. In particular, all structures in $\mathfrak{F}_d$ are d-bounded.

Theorem 9.3.1. *Let $d \geq 2$. There is no algorithm that computes, on input of a sentence φ from $\mathsf{FO}[\tau_d]$, in time*

$$2^{2^{o(||\varphi||)}} \quad \textit{for } d = 2, \qquad \textit{and in time} \quad 2^{d^{2^{o(||\varphi||)}}} \quad \textit{for } d \geq 3$$

a HNF*-sentence from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ that is equivalent to φ on $\mathfrak{F}_d$.*

Theorem 9.3.1 follows directly from Corollary 9.2.2 and the following lemma, where we construct suitable sequences of "small" formulae for which we show lower bounds on the size of d-equivalent HNF-sentences. The proof of Lemma 9.3.2 is provided in Section 9.3.2. It follows the basic idea of the lower bound from [BK12]. Its key combinatorial argument is stated and proven in Section 9.3.1 below.

Lemma 9.3.2. *Let $d \geq 2$ be a degree bound. There is a number $c_d \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_{d,h})_{h \geq 1}$ of $\mathsf{FO}[\tau_d]$-sentences such that for every $h \geq 1$,*

(1) $||\varphi_{d,h}|| \leq c_d \cdot h$, and

(2) every HNF*-sentence in $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ that is $\mathfrak{F}_d$-equivalent to $\varphi_{d,h}$ has size $\geq |\mathfrak{T}_{d,2^h}|$.*

9.3.1 The Combinatorial Argument

In the following, we call a set $\mathfrak{D}$ of structures *substructure-free* if no proper induced substructure of a structure in $\mathfrak{D}$ is also contained in $\mathfrak{D}$. Observe that, in particular, the sets $\mathfrak{T}_{d,h}$ for degree bounds $d \geq 2$ and $h \geq 0$ are substructure-free.

Lemma 9.3.3. *Let σ be a relational signature and let $\mathfrak{C}$ be a class of σ-structures that is closed under disjoint unions and induced substructures. Let $\mathfrak{D}$ be a finite substructure-free subset of $\mathfrak{C}$ such that each structure in $\mathfrak{D}$ has at least two elements and a connected Gaifman graph, and such that all structures in $\mathfrak{D}$ are pairwise non-isomorphic.*

Suppose that there is a sentence φ in $\mathsf{FO}[\sigma]$ such that for every $\mathcal{A} \in \mathfrak{C}$,

$$\mathcal{A} \models \varphi$$

iff $\quad \mathcal{A}$ contains at most one disjoint copy of each structure from $\mathfrak{D}$.

Then, every HNF*-sentence ψ in $\mathsf{FO{+}unT}[\sigma]$ that is equivalent to φ on $\mathfrak{C}$ contains at least $|\mathfrak{D}|$ counting-sentences and thus, $||\psi|| > |\mathfrak{D}|$.*

Proof. Let σ be a relational signature and let $\mathfrak{C}$ be a class of σ-structures that is closed under disjoint unions and induced substructures. Let $\mathfrak{D}$ be a finite substructure-free subset of $\mathfrak{C}$ such that each structure in $\mathfrak{D}$ has at least two elements and a connected Gaifman graph, and such that all structures in $\mathfrak{D}$ are pairwise non-isomorphic.

For a contradiction, assume that $\psi \in \mathsf{FO{+}unT}[\sigma]$ is a HNF-sentence that is equivalent to φ on $\mathfrak{C}$ and that contains less than $|\mathfrak{D}|$ counting-sentences.

Then, there has to be a structure $\mathcal{C} \in \mathfrak{D}$, such that for every counting-sentence $\exists^{\geq k} y\ \mathrm{sph}_\tau(y)$ that occurs in ψ,

$$\tau \ \not\cong\ (\mathcal{C}, c) \quad \text{for every } c \in C. \tag{1}$$

In the following, we choose $K \geq 1$ and $R \geq 0$, such that each counting-sentence $\exists^{\geq k} y\ \mathrm{sph}_\tau(y)$ in ψ has $k \leq K$ and a type τ of radius $r \leq R$.

Let $\mathcal{A} \in \mathfrak{C}$ be the disjoint union of K copies of all *proper* induced substructures $\mathcal{C}[N_r^{\mathcal{C}}(c)]$ of $\mathcal{C}$ with $c \in C$ and $r \leq R$ (such structures exist since $\mathcal{C}$ has at least two elements). Since $\mathfrak{D}$ is substructure-free and all structures in $\mathfrak{D}$ have a connected Gaifman graph, $\mathcal{A}$ does not contain any structure from $\mathfrak{D}$ as an induced substructure.

Furthermore, let $\mathcal{B} \in \mathfrak{C}$ be the disjoint union of $\mathcal{A}$ with two copies of the structure $\mathcal{C}$. By choice of φ, we have that

$$\mathcal{A} \models \varphi \qquad \text{and} \qquad \mathcal{B} \not\models \varphi .$$

Since ψ is equivalent to φ on $\mathfrak{C}$, we furthermore have

$$\mathcal{A} \models \psi \qquad \text{and} \qquad \mathcal{B} \not\models \psi . \tag{2}$$

We complete the proof of Lemma 9.3.3 by showing that

$$\mathcal{A} \models \psi \qquad \text{iff} \qquad \mathcal{B} \models \psi , \tag{3}$$

which, obviously, is a contradiction to Statement (2).

Consider an arbitrary counting-sentence $\chi := \exists^{\geq k} y \ \mathrm{sph}_\tau(y)$ from ψ. Note that $k \in [1, K]$ and τ is a type of radius $r \leq R$. We will show that

$$\mathcal{A} \models \chi \qquad \text{iff} \qquad \mathcal{B} \models \chi . \tag{4}$$

Since $\mathcal{B}$ is a disjoint extension of $\mathcal{A}$, the *"only if" direction* of Equivalence (4) is obvious. For the *"if" direction*, assume towards a contradiction that

$$\mathcal{A} \not\models \chi \qquad \text{and} \qquad \mathcal{B} \models \chi .$$

Since, by definition of χ, this implies that

$$|\{a \in A : \mathcal{N}_r^{\mathcal{A}}(a) \cong \tau\}| \ < \ k \quad \text{and} \quad |\{b \in B : \mathcal{N}_r^{\mathcal{B}}(b) \cong \tau\}| \ \geq \ k , \tag{5}$$

we can conclude that there is a $c \in C$ such that $\tau \cong \mathcal{N}_r^{\mathcal{C}}(c)$. Recall that, by Statement (1), $\tau \not\cong (\mathcal{C}, c)$. But then, by construction of $\mathcal{A}$, the structure $\mathcal{A}$ contains at least K copies of $\mathcal{C}[N_r^{\mathcal{C}}(c)]$ as disjoint substructures. This is a contradiction to the left side of Statement (5). Thus, $\mathcal{A} \models \chi$.

We can conclude that Equivalence (3) holds, which is a contradiction to Statement (2). This completes the proof of Lemma 9.3.3. □

9.3.2 Small Sentences with Large Hanf Normal Form Sentences

In this section, we prove Lemma 9.3.2. To this aim, recall that for each degree bound $d \geq 2$, the class $\mathfrak{F}_d$ is closed under disjoint unions and induced substructures. Furthermore, for each $h \geq 1$, the set $\mathfrak{T}_{d,2^h}$ is substructure-free, all structures in the set are pairwise non-isomorphic, and each structure in $\mathfrak{T}_{d,2^h}$ has more than two elements and a connected Gaifman graph.

Proof of Lemma 9.3.2 using Lemma 9.3.3. Let $d \geq 2$ be a degree bound. Using the formulae provided by Lemma 9.2.3, we let, for each $h \geq 1$,

$$\varphi_{d,h} \ \coloneqq \ \forall x \forall y \Big((\mathrm{root}_{d,h}(x) \ \wedge \ \mathrm{root}_{d,h}(y) \ \wedge \ \neg x{=}y) \ \rightarrow \ \neg\, \mathrm{iso}_{d,h}(x,y) \Big)$$

with the subformula

$$\mathrm{root}_{d,h}(x) \ \coloneqq \ \neg \exists y \bigvee_{j=0}^{d-2} S_j(x,y) \ \wedge \ \mathrm{complete}_{d,h}(x).$$

By this definition, it holds for every $\mathcal{A} \in \mathfrak{F}_d$ that

$\mathcal{A} \models \varphi_{d,h}$

iff $\mathcal{A}$ contains at most one disjoint copy of each structure from $\mathfrak{T}_{d,2^h}$.

By Lemma 9.2.3, there is a number $c_d \in \mathbb{N}_{\geq 1}$ such that for all $h \geq 1$, the sentence $\varphi_{d,h}$ has size $\leq c_d \cdot h$. Therefore, it follows from Lemma 9.3.3 that each HNF-sentence in $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ that is $\mathfrak{F}_d$-equivalent to $\varphi_{d,h}$ has size at least $|\mathfrak{T}_{d,2^h}|$. This completes the proof of Lemma 9.3.2. $\square$

9.4 Gaifman Normal Form

In this section, we show that the algorithm of Theorem 4.1.7 for the construction of Gaifman normal form on classes of structures of bounded degree is basically worst-case optimal.

For the statement of the first main result of this section, recall that $\mathfrak{T}_d$, for $d \geq 3$, is the class of labelled and ordered trees of arity $d-1$ (cf. Section 9.2.1).

Theorem 9.4.1. *Let $d \geq 3$ be a degree bound. There is no algorithm that computes, on input of a sentence φ from $\mathsf{FO}[\tau_d]$, in time*

$$2^{d^{2^{o(||\varphi||)}}}$$

a GNF*-sentence from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ that is $\mathfrak{T}_d$-equivalent to φ.*

For the specific case of degree bound 3, we can show the following lower bound on the class $\mathfrak{BT}$ of binary trees (cf. Section 9.2.3) over the signature (E).

Theorem 9.4.2. *There is no algorithm that computes, on input of a sentence φ from $\mathsf{FO}[E]$, in time*

$$2^{2^{2^{o(||\varphi||)}}}$$

a GNF*-sentence from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[E]$ that is $\mathfrak{BT}$-equivalent to φ.*

For degree bound 2, recall from Section 9.2.2 that $\mathfrak{T}_2$ is the class of all labelled chains.

Theorem 9.4.3. *There is no algorithm that computes, on input of a sentence φ from $\mathsf{FO}[\tau_2]$, in time*

$$2^{2^{o(||\varphi||)}}$$

a GNF*-sentence from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_2]$ that is $\mathfrak{T}_2$-equivalent to φ.*

The proofs for the lower bounds stated in Theorem 9.4.1, Theorem 9.4.2, and Theorem 9.4.3 are based on the proof of Theorem 4.2 in [DGKS07], where the tree encoding recalled in Section 9.2.3 is used for a non-elementary lower bound on the size of Gaifman normal forms on the class $\mathfrak{T}$ of trees.

In Section 9.4.1, a game is presented that distills the basic idea of the latter lower bound of [DGKS07] in the shape of a game. Section 9.4.2 presents as Theorem 9.4.5 a straightforward application of the game for lower bounds on classes of structures that are closed under disjoint unions (e.g., forest-like structures). There, we also show a slight improvement of the non-elementary lower bound of [DGKS07] with respect to the class of forests of arbitrary degree, which can be generalised to the class of trees.

The following sections are devoted to the proofs of Theorem 9.4.1, Theorem 9.4.2, and Theorem 9.4.3. Although similar to the proof of Theorem 9.4.5, considerably more care is needed in the construction of the lower bounds on classes of connected structures.

9.4.1 A Game Characterisation

Let σ be a relational signature, let $\mathfrak{C}$ be a class of σ-structures, and let φ be an $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$-sentence.

For each $H \geq 1$, the H-game for φ on $\mathfrak{C}$ has three rounds and is played between two players, called Spoiler and Duplicator. The idea behind the game is that for any GNF-sentence ψ of size $< H$, Duplicator tries to find structures $\mathcal{A}, \mathcal{B} \in \mathfrak{C}$ which can be distinguished by φ, but not by ψ.

In particular, Duplicator can choose $\mathcal{A}$ an $\mathcal{B}$ depending on the locality radius of the local formulae in the basic local sentences of ψ. This will be useful if $\mathfrak{C}$ is a class of structures that is not closed under disjoint unions as, e.g., the class of binary trees.

(Round 1) *Spoiler* chooses a number $r \geq 0$.

Duplicator chooses a structure $\mathcal{A} \in \mathfrak{C}$.

If $\mathcal{A} \models \varphi$, the game continues. Otherwise, Spoiler wins.

(Round 2) *Spoiler* chooses a tuple $\overline{a} \in A^n$ of length $n \in [1, H)$.

Duplicator chooses a structure $\mathcal{B} \in \mathfrak{C}$ and a tuple $\overline{b} \in B^n$.

If $\mathcal{B} \not\models \varphi$ and $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \mathcal{N}_r^{\mathcal{B}}(\overline{b})$, the game continues.
Otherwise, Spoiler wins.

(Round 3) *Spoiler* chooses a number $s \leq r$ and
a $2s$-scattered tuple $\overline{b} \in B^n$ of length $n \in [1, H)$.

Duplicator chooses a tuple $\overline{a} \in A^n$.

If $\mathcal{N}_s^{\mathcal{A}}(\overline{a}) \cong \mathcal{N}_s^{\mathcal{B}}(\overline{b})$, Duplicator wins. Otherwise, Spoiler wins.

In the description of the game, a tuple $(b_1, \ldots, b_n) \in B^n$ of length $n \geq 0$ of elements from the universe of a σ-structure $\mathcal{B}$ is called *s-scattered*, for an $s \geq 0$, if the nodes $b_1, \ldots, b_n$ are pairwise distinct and, furthermore, have pairwise distance $> s$ in the Gaifman graph $\mathcal{G}_{\mathcal{B}}$ of $\mathcal{B}$.

Duplicator has a *winning strategy* in the H-game for φ on $\mathfrak{C}$, if he can win the game for all possible choices of Spoiler in Rounds (1) to (3). The following lemma shows that this implies a lower bound on the size of Gaifman normal forms on $\mathfrak{C}$.

Lemma 9.4.4. *For every relational signature σ, each class $\mathfrak{C}$ of σ-structures, every $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$-sentence φ, and each $H \geq 1$, the following holds: If Duplicator has a winning strategy in the H-game for φ on $\mathfrak{C}$, then every* GNF*-sentence from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ that is $\mathfrak{C}$-equivalent to φ has size $\geq H$.*

Proof. Let σ be a relational signature and let $\mathfrak{C}$ be a class of σ-structures. Let φ be an $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$-sentence and let $H \geq 1$ such that Duplicator has a winning strategy in the H-game for φ on $\mathfrak{C}$.

For a contradiction, assume that there is a GNF-sentence ψ in $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ with size $< H$ that is $\mathfrak{C}$-equivalent to φ. That is, for each $\mathcal{A} \in \mathfrak{C}$, we have

$$\mathcal{A} \models \varphi \quad \text{iff} \quad \mathcal{A} \models \psi. \tag{1}$$

Being a GNF-sentence, ψ is a Boolean combination of basic local sentences $\chi_1, \dots, \chi_L$, for an $L \geq 1$, where each basic local sentence χ_ℓ is of the shape

$$\exists x_1 \cdots \exists_{k_\ell} \underbrace{\Bigg(\bigwedge_{1 \leq i < j \leq k_\ell} \operatorname{dist}(x_i, x_j) > 2r_\ell \ \wedge \ \bigwedge_{i=1}^{k_\ell} \varrho_\ell(x_i) \Bigg)}_{\delta_\ell(x_1, \dots, x_{k_\ell})}$$

for numbers $k_\ell, r_\ell \geq 1$ and a formula $\varrho_\ell(x)$ that is r_ℓ-local around x. For each $\ell \in [1, L]$, we denote by $\delta_\ell(x_1, \dots, x_{k_\ell})$ the subformula of χ_ℓ without the quantifier prefix $\exists x_1 \cdots \exists x_{k_\ell}$.

In the rest of the proof, we will use the winning strategy for Duplicator in the H-game for φ on $\mathfrak{C}$ to obtain structures $\mathcal{A}, \mathcal{B} \in \mathfrak{C}$ which can be distinguished by φ but not by ψ — which immediately leads to a contradiction to the assumption stated in Equivalence (1).

In Round (1), let Spoiler choose the number $r := \max\{r_1, \dots, r_\ell\}$, that is, the maximum of the radii of the local formulae in the basic local sentences of ψ. Duplicator's winning strategy provides a structure $\mathcal{A} \in \mathfrak{C}$ such that $\mathcal{A} \models \varphi$. Since φ and ψ are, by assumption, $\mathfrak{C}$-equivalent, also $\mathcal{A} \models \psi$.

The following claim implies that there is a structure $\mathcal{B} \in \mathfrak{C}$ such that $\mathcal{B} \not\models \varphi$ but $\mathcal{B} \models \psi$, completing the proof of Lemma 9.4.4.

Claim 1. *There is a structure $\mathcal{B} \in \mathfrak{C}$ such that $\mathcal{B} \not\models \varphi$ and for each $\ell \in [1, L]$,*

$$\mathcal{A} \models \chi_\ell \quad \textit{iff} \quad \mathcal{B} \models \chi_\ell.$$

For the proof of Claim 1, we make use of Duplicator's winning strategy for Round (2) and Round (3).

Proof of Claim 1. Without loss of generality, there is an $\tilde{L} \in [0, L]$ such that

$$\mathcal{A} \models \chi_\ell \quad \text{for all } \ell \leq \tilde{L}, \quad \text{and} \quad \mathcal{A} \not\models \chi_\ell \quad \text{for all } \ell > \tilde{L}. \tag{2}$$

For all $\ell \in [1, \tilde{L}]$, we know by Statement (2) that $\mathcal{A} \models \chi_\ell$. Hence, for each $\ell \in [1, \tilde{L}]$, there is a tuple $\overline{a} \in A^{k_\ell}$ such that $\mathcal{A} \models \delta_\ell[\overline{a}]$. Let $\overline{a} := (\overline{a}_1, \dots, \overline{a}_{\tilde{L}})$ the concatenation of all these tuples. Clearly, the length $n := k_1 + \cdots + k_{\tilde{L}}$ of $\overline{a}$ is less than $||\psi||$ and thus less than H.

In Round (2), let Spoiler choose the tuple $\overline{a}$ just defined. Duplicator's winning strategy provides us with a structure $\mathcal{B} \in \mathfrak{C}$ with $\mathcal{B} \not\models \varphi$ and a tuple $\overline{b} \in B^n$ such that $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \mathcal{N}_r^{\mathcal{B}}(\overline{b})$. For every $\ell \in [1, \tilde{L}]$, let $\overline{b}_\ell \in B^{k_\ell}$ such that $\overline{b} = (\overline{b}_1, \dots, \overline{b}_{\tilde{L}})$.

In particular, we have $\mathcal{N}_r^{\mathcal{A}}(\bar{a}_\ell) \cong \mathcal{N}_r^{\mathcal{B}}(\bar{b}_\ell)$ for each $\ell \in [1, \tilde{L}]$. Since $r_\ell \leq r$, it follows, that $\mathcal{B} \models \delta_\ell[\bar{b}_\ell]$ and hence, $\mathcal{B} \models \chi_\ell$ for all $\ell \in [1, \tilde{L}]$.

For each $\ell \in [\tilde{L}+1, L]$, we know that $\mathcal{A} \not\models \chi_\ell$, and we want to show that also $\mathcal{B} \not\models \chi_\ell$. Towards a contradiction, assume that $\mathcal{B} \models \chi_\ell$. That is, assume that there is a tuple $\bar{b} \in B^{k_\ell}$ such that $\mathcal{B} \models \delta_\ell[\bar{b}]$. Of course, $k_\ell < H$. Furthermore, by construction of $\delta_\ell(x_1, \ldots, x_{k_\ell})$, the tuple $\bar{b}$ is $2r_\ell$-scattered for $r_\ell \leq r$.

In Round (3), let Spoiler choose the number r_ℓ and the $2r_\ell$-scattered tuple $\bar{b}$ just defined. Duplicator's winning strategy provides a tuple $\bar{a} \in A^{k_\ell}$ with $\mathcal{N}_{r_\ell}^{\mathcal{A}}(\bar{a}) \cong \mathcal{N}_{r_\ell}^{\mathcal{B}}(\bar{b})$. Therefore, $\mathcal{A} \models \delta_\ell[\bar{a}]$ and hence, $\mathcal{A} \models \chi_\ell$. This, however, is a contradiction to the assumption that $\mathcal{A} \not\models \chi_\ell$. It follows that $\mathcal{B} \not\models \chi_\ell$.

This completes the proof of Claim 1 and also the proof of Lemma 9.4.4. □

The following section presents a straightforward application of Lemma 9.4.4 to prove lower bounds on the size of Gaifman normal forms with respect to classes of structures that are closed under disjoint unions.

9.4.2 Lower Bounds for Classes Closed Under Disjoint Unions

As an easy example for the application of Lemma 9.4.4, we consider classes of structures that are closed under disjoint unions in this section. Precisely, we show the following variation of Theorem 9.4.1, which is a weaker statement in the sense that the stated lower bounds are not over classes of tree-like but forest-like structures. On the other hand, it also includes a lower bound for degree bound 2.

For the first result of this section, recall from Section 9.2.1 that $\mathfrak{F}_d$ is the class of all labelled and ordered forests of degree $d-1$.

Theorem 9.4.5. *Let $d \geq 2$ be a degree bound. There is no algorithm that computes, on input of a sentence φ from $\mathsf{FO}[\tau_d]$, in time*

$$2^{2^{o(||\varphi||)}} \quad \textit{for } d = 2, \qquad \textit{and in time} \quad 2^{d^{2^{o(||\varphi||)}}} \quad \textit{for } d \geq 3$$

a GNF*-sentence from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ that is $\mathfrak{F}_d$-equivalent to φ.*

In the same manner as Theorem 9.4.5, we can also improve the lower bound of Theorem 4.3 in [DGKS07] for classes of forests of bounded height (without any restriction to the degree). For each $h \geq 0$, we denote by $\mathfrak{F}_{\leq h}$ the class of all forests of height $\leq h$ from $\mathfrak{F}$.

Theorem 9.4.6. *There is a sequence* $(\varphi_h)_{h\geq 1}$ *of* $\mathsf{FO}[E]$*-sentences of size* $\mathcal{O}(h)$ *such that, for each* $h \geq 1$*, every* GNF*-sentence from* $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[E]$ *that is equivalent to* φ *on* $\mathfrak{F}_{\leq h}$ *has size* $\geq \mathrm{Tower}(h)$*.*

For comparison, the sequence of $\mathsf{FO}[E]$-sentences provided by Theorem 4.3 of [DGKS07] has the same lower bound on the size of $\mathfrak{F}_{\leq h}$-equivalent GNF-sentences for each $h \geq 1$ but its sentences have size in $\Omega(h^4)$. The reason for this is that the sentences make use of sub-formulae expressing arithmetic over tree encodings.

The following application of Lemma 9.4.4 shows that there are simpler sentences, which do not use arithmetic over tree encodings, that have large equivalent GNF-sentences (with respect to a class of structures). The lemma will be used in the proofs of Theorem 9.4.5 and Theorem 9.4.6.

Lemma 9.4.7. *Let* σ *be a relational signature and let* $\mathfrak{C}$ *be a class of structures over the signature* σ *that is closed under disjoint unions. Let* $\mathfrak{D}$ *be a non-empty finite set pairwise non-isomorphic structures from* $\mathfrak{C}$*.*

Suppose that φ *is a sentence from* $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ *such that for every* $\mathcal{A} \in \mathfrak{C}$*,*

$$\mathcal{A} \models \varphi$$

iff *no structure* $\mathcal{D} \in \mathfrak{D}$ *has precisely one disjoint copy in* $\mathcal{A}$*.*

Then, each GNF*-sentence in* $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ *that is* $\mathfrak{C}$*-equivalent to* φ *has size* $\geq |\mathfrak{D}|$*.*

Proof. Let σ be a relational signature, let $\mathfrak{C}$ be a class of σ-structures that is closed under disjoint unions, and let $\mathfrak{D}$ be a non-empty finite set of pairwise non-isomorphic structures from $\mathfrak{C}$. Furthermore, suppose that φ is a sentence from $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ such that any structure $\mathcal{A} \in \mathfrak{C}$ is a model of φ if and only if no structure $\mathcal{D} \in \mathfrak{D}$ has precisely one disjoint copy in $\mathcal{A}$. Let $H := |\mathfrak{D}|$.

In the following, we will show that Duplicator has a winning strategy in the H-game for φ on $\mathfrak{C}$, and thus, by Lemma 9.4.4, each GNF-sentence in $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ that is $\mathfrak{C}$-equivalent to φ has size $\geq H$.

Let $\mathcal{A}$ be the disjoint union of two copies of each structure from $\mathfrak{D}$. By assumption on φ, $\mathcal{A} \models \varphi$. For each $\mathcal{D} \in \mathfrak{D}$, we let $\mathcal{A}^{-\mathcal{D}}$ be the induced substructure of $\mathcal{A}$ obtained by removing *one* disjoint copy of the structure $\mathcal{D}$ from $\mathcal{A}$. Clearly, $\mathcal{A}^{-\mathcal{D}} \not\models \varphi$.

Duplicator wins the H-game for φ on $\mathfrak{C}$ by the following winning strategy.

Round (1). Independent of Spoiler's choice of $r \geq 0$, Duplicator replies with the structure $\mathcal{A}$ defined above.

Round (2). Let $\overline{a} \in A^n$ with $n \in [1, H)$ be the tuple chosen by Spoiler. As $|\mathfrak{D}| > n$, there is a structure $\mathcal{D} \in \mathfrak{D}$ such that none of the elements of $\overline{a}$ belongs to one of the copies of $\mathcal{D}$ in $\mathcal{A}$. Duplicator replies with the structure $\mathcal{A}^{-\mathcal{D}}$ and with the same tuple $\overline{a}$. Clearly, $\mathcal{N}_r^{\mathcal{A}}(\overline{a}) \cong \mathcal{N}_r^{\mathcal{A}^{-\mathcal{D}}}(\overline{a})$. Furthermore, by construction of φ, $\mathcal{A}^{-\mathcal{D}} \not\models \varphi$.

Round (3). Suppose that Spoiler chooses $s \leq r$ and a $2s$-scattered tuple $\overline{b}$ from $A^{-\mathcal{D}}$ of length $n \in [1, H)$. Recall that $\mathcal{A}^{-\mathcal{D}}$ is an induced substructure of $\mathcal{A}$ and that each disjoint substructure of $\mathcal{A}^{-\mathcal{D}}$ is, without any modifications, also present in $\mathcal{A}$. Thus, we have $\mathcal{N}_s^{\mathcal{A}}(\overline{b}) \cong \mathcal{N}_s^{\mathcal{A}^{\mathcal{D}}}(\overline{b})$. Duplicator replies with the same tuple $\overline{b}$.

This completes the proof of Lemma 9.4.7. ☐

Theorem 9.4.5 is a direct consequence of Corollary 9.2.2 and the following lemma, which, for each $d \geq 2$, uses Lemma 9.4.7 to provide lower bounds on the size of $\mathfrak{F}_d$-equivalent GNF-sentences for a sequence of sentences from $\mathsf{FO}[\tau_d]$.

Lemma 9.4.8. *Let $d \geq 2$ be a degree bound. There is a number $c_d \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_{d,h})_{h\geq 1}$ of $\mathsf{FO}[\tau_d]$-sentences such that for every $h \geq 1$,*

(1) $||\varphi_{d,h}|| \leq c_d \cdot h$, *and*

(2) every GNF*-sentence in* $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ *that is $\mathfrak{F}_d$-equivalent to $\varphi_{d,h}$ has size* $\geq |\mathfrak{T}_{d,2^h}|$.

Proof. Let $d \geq 2$ be a degree bound. For each $h \geq 1$, let

$$\varphi_{d,h} \;:=\; \forall x \Big(\mathrm{root}(x) \;\rightarrow\; \exists y \left(\mathrm{root}(y) \;\wedge\; \mathrm{iso}_{d,h}(x,y) \;\wedge\; \neg x{=}y\right)\Big)$$

with $\mathrm{root}(x) := \neg\exists y\, E(y,x)$. By construction of $\varphi_{d,h}$, it holds that for every disjoint union $\mathcal{A}$ of structures from the set $\mathfrak{T}_{d,2^h}$,

$$\mathcal{A} \models \varphi_{d,h}$$

iff no $\mathcal{T} \in \mathfrak{T}_{d,2^h}$ has precisely one disjoint copy in $\mathcal{A}$.

Since all disjoint unions of structures from $\mathfrak{T}_{d,2^h}$ belong to $\mathfrak{F}_d$, it follows from Lemma 9.4.7 that every GNF-sentence in $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ that is $\mathfrak{F}_d$-equivalent to $\varphi_{d,h}$ has size $\geq |\mathfrak{T}_{d,2^h}|$. This completes the proof of Lemma 9.4.8. ☐

We conclude the section with the proof of Theorem 9.4.6.

Proof. The proof is very similar to the one of Lemma 9.4.8 but uses the encoding of numbers by trees over the signature (E), introduced in the first part of Section 9.2.3. For each $h \geq 1$, let

$$\varphi_h \;\coloneqq\; \forall x \Big(\mathrm{root}(x) \;\to\; \exists y \left(\mathrm{root}(y) \;\wedge\; \mathrm{eq}_h(x,y) \;\wedge\; \neg x{=}y \right) \Big)$$

with $\mathrm{root}(x) \coloneqq \neg\exists y\, E(y,x)$ and the formula $\mathrm{eq}_h(x,y)$ provided by Lemma 9.2.6. Clearly, there is a number $c \in \mathbb{N}_{\geq 1}$ such that $||\varphi_h|| \leq c \cdot h$ for each $h \geq 1$.

Let $h \geq 1$ and let $\mathfrak{T}(h)$ denote the set of all tree encodings $\mathcal{T}(i)$ for all numbers $i \in [0, \mathrm{Tower}(h))$. For every disjoint union $\mathcal{A}$ of trees from $\mathfrak{T}(h)$ it is straightforward to verify that

$$\mathcal{A} \models \varphi_h$$

iff no tree from $\mathfrak{T}(h)$ has precisely one disjoint copy in $\mathcal{A}$.

Since all disjoint unions of trees from $\mathfrak{T}(h)$ belong to $\mathfrak{F}_{\leq h}$, it follows from Lemma 9.4.7 that every GNF-sentence in $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[E]$ which is equivalent to φ_h on $\mathfrak{F}_{\leq h}$ has size $\geq |\mathfrak{T}(h)| = \mathrm{Tower}(h)$. $\square$

9.4.3 Ordered and Labelled Trees of Bounded Degree

This section is devoted to the proof of Theorem 9.4.1, which is implied by Corollary 9.2.2 and the following lemma. The lemma uses the idea of the proof of Theorem 4.2 in [DGKS07].

Lemma 9.4.9. *Let $d \geq 3$ be a degree bound. There is a number $c_d \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_{d,h})_{h \geq 1}$ of $\mathsf{FO}[\tau_d]$-sentences such that for every $h \geq 1$,*

(1) $||\varphi_{d,h}|| \leq c_d \cdot h$, and

(2) every GNF-sentence in $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ that is $\mathfrak{T}_d$-equivalent to $\varphi_{d,h}$ has size $\geq |\mathfrak{T}_{d,2^h}|$.

Proof. Let $d \geq 3$ be a degree bound. Let $h \geq 1$ and let $H \coloneqq |\mathfrak{T}_{d,2^h}|$. For each $R \geq 6$, we define the following τ_d-structures:

- $\mathcal{C}_{h,R}$ is a path of S_0-edges along nodes $a_0, \ldots, a_{(2H+1)R}$, that is, the τ_d-structure with universe $\{a_0, \ldots, a_{(2H+1)R}\}$ and where for all $i, j \in [0, (2H{+}1)R]$, the tuple (a_i, a_j) belongs to $S_0^{\mathcal{C}_{h,R}}$ if and only if $j = i + 1$. The other successor relations $S_j^{\mathcal{C}_{h,R}}$ for $j \in [1, d{-}2]$ are empty.

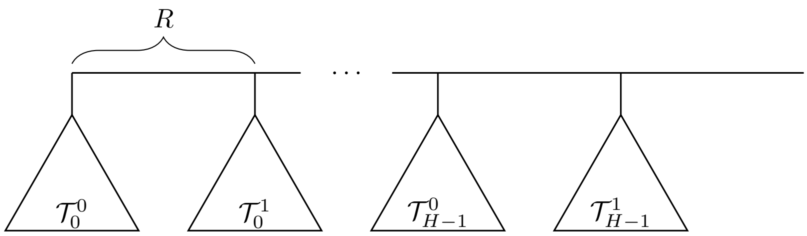

Figure 9.3 The structure $\mathcal{T}_{h,R}$.

- For each $i \in [0, H)$ and every $j \in \{0, 1\}$, $\mathcal{T}_i^j$ denotes a τ_d-structure whose universe is disjoint to the universe of $\mathcal{C}_{h,R}$. Moreover, the universes of all $\mathcal{T}_i^j$ for all $i \in [0, H)$ and $j \in \{0, 1\}$ are pairwise disjoint. Furthermore, for all $i \in [0, H)$, $\mathcal{T}_i^0$ and $\mathcal{T}_i^1$ are isomorphic and, for each $\mathcal{T} \in \mathfrak{T}_{d,2^h}$, there is precisely one $i \in [0, H)$ such that $\mathcal{T}_j^0$ as well as $\mathcal{T}_j^1$ are isomorphic to $\mathcal{T}$.
- The structure $\mathcal{T}_{h,R} \in \mathfrak{T}_d$ is obtained by attaching all $\mathcal{T}_i^j$ with $i \in [0, H)$ and $j \in \{0, 1\}$ to nodes of the path $\mathcal{C}_{h,R}$ which have distance at least R to each other (see Figure 9.3 for an illustration). More precisely, $\mathcal{T}_{h,R}$ is build from the union of $\mathcal{C}_{h,R}$ with all $\mathcal{T}_i^j$ for all $i \in [0, H)$ and $j \in \{0, 1\}$, and for each $i \in [0, H)$ and $j \in \{0, 1\}$, there is an additional edge in the successor relation $\mathcal{S}_1^{\mathcal{T}_{h,R}}$ from the node $a_{(2i+j)R}$ on the path to the root node of $\mathcal{T}_i^j$.
- For each $k \in [0, H)$, we denote by $\mathcal{T}_{h,R}^{-k}$ the structure $\mathcal{T}_{h,R} - T_k^0$, that is, the substructure of $\mathcal{T}_{h,R}$ induced by removing all the nodes that belong to the universe of $\mathcal{T}_k^0$.

We will now define $\mathsf{FO}[\tau_d]$-sentences $\varphi_{d,h}$ for $h \geq 1$ that have size $\mathcal{O}(h)$ and for which Duplicator has a winning strategy in the H-game on $\mathfrak{T}_d$. The basic idea of the sentences will be similar to the corresponding sentence in the proof of Lemma 9.4.8.

Claim 1. *There is a number $c_d \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_{d,h})_{h \geq 1}$ of sentences from $\mathsf{FO}[\tau_d]$ such that for each $h \geq 1$, $||\varphi_{d,h}|| \leq c_d \cdot h$, and for all $R \geq 6$,*

$$\mathcal{T}_{h,R} \models \varphi_{d,h} \quad \textit{and} \quad \mathcal{T}_{h,R}^{-k} \not\models \varphi_{d,h} \quad \textit{for all } k \in [0, H). \tag{1}$$

Proof of Claim 1. We first have to find an $\mathsf{FO}[\tau_d]$-formula that recognises the roots of the structures $\mathcal{T}_i^j$ in the structures $\mathcal{T}_{h,R}$ and $\mathcal{T}_{h,R}^{-k}$ for all $k \in [0, H)$. Recall that all structures in $\mathfrak{T}_{d,2^h}$ are complete with height 2^h. Thus, by construction of $\mathcal{T}_{h,R}$

and $\mathcal{T}_{h,R}^{-k}$, the roots of the $\mathcal{T}_i^j$ are precisely the nodes satisfying the formula $\text{complete}_{d,h}(x)$ provided by Lemma 9.2.3.

With this, it is straightforward to verify that, for each $h \geq 1$, the sentence

$$\varphi_{d,h} \;\coloneqq\; \forall x \Big(\text{complete}_{d,h}(x) \;\rightarrow\; \exists y \left(\text{complete}_{d,h} \;\wedge\; \text{iso}_{d,h}(x,y) \;\wedge\; \neg x{=}y\right)\Big).$$

satisfies Statement (1). Furthermore, by Lemma 9.2.3, there is a number $c_d \in \mathbb{N}_{\geq 1}$ such that $||\varphi_{d,h}|| \leq c_d \cdot h$ for all $h \geq 1$. This completes the proof of Claim 1.

By Lemma 9.4.4, it suffices to prove the following claim to complete the proof of Lemma 9.4.9.

Claim 2. *For each $h \geq 1$, Duplicator has a winning strategy in the H-game for $\varphi_{d,h}$ on $\mathfrak{T}_d$.*

Proof of Claim 2. Let $h \geq 1$. We describe a winning strategy for Duplicator in the H-game for $\varphi_{d,h}$ on $\mathfrak{T}_d$.

Round (1). Suppose that Spoiler chooses the radius $r \geq 0$. For the following, let

$$R \;\coloneqq\; 4 + \max\{2, 4r\}.$$

By Statement (1), Duplicator can reply with the tree $\mathcal{T}_{h,R}$ to win this round.

Round (2). Let $\overline{a}$ be the tuple of elements from $\mathcal{T}_{h,R}$ which Spoiler chooses in this round, and let $n \in [1, H)$ be the length of this tuple.

By construction, $\mathcal{T}_{h,R}$ contains all the trees $\mathcal{T}_i^0$ for all $i \in [0, H)$. Furthermore, for all $i, j \in [0, H)$, each node a from $\mathcal{T}_i^0$ and each node b from $\mathcal{T}_j^0$ have pairwise distance $\geq R + 2$. Thus, there has to be a number $k \in [0, H)$ such that none of the elements of $\overline{a}$ belongs to the subtree $\mathcal{T}_k^0$ of $\mathcal{T}_{h,R}$, and also not to the $(R/2)$-neighbourhood of the nodes of $\mathcal{T}_k^0$ in $\mathcal{T}_{h,R}$.

Duplicator replies with the structure $\mathcal{T}_{h,R}^{-k}$ and with the same tuple $\overline{a}$. Recall that, by Statement (1), $\mathcal{T}_{h,R}^{-k} \not\models \varphi_{d,h}$. Furthermore, since $R/2 > 2r$, also

$$\mathcal{N}_r^{\mathcal{T}_{h,R}}(\overline{a}) \;\cong\; \mathcal{N}_r^{\mathcal{T}_{h,R}^{-k}}(\overline{a}).$$

Thus, Duplicator wins the round.

Round (3). Let $s \leq r$ be the radius chosen by Spoiler, let $\overline{b}$ be the $2s$-scattered tuple of nodes from $\mathcal{T}_{h,R}^{-k}$ chosen by Spoiler, and let $n \in [1, H)$ be the length of $\overline{b}$. Recall that Duplicator has to reply with a tuple $\overline{a}$ of the same length n of nodes from $\mathcal{T}_{h,R}$ such that

$$\mathcal{N}_s^{\mathcal{T}_{h,R}}(\overline{a}) \;\cong\; \mathcal{N}_s^{\mathcal{T}_{h,R}^{-k}}(\overline{b}). \tag{2}$$

Of course, each of the nodes in $\overline{b}$ also occurs in $\mathcal{T}_{h,R}$ and the pairwise distance of these nodes is the same as in $\mathcal{T}_{h,R}^{-k}$ and thus $> 2s$. If furthermore the s-spheres of all nodes in $\overline{b}$ are the same in $\mathcal{T}_{h,R}$ and $\mathcal{T}_{h,R}^{-k}$, Duplicator satisfies Isomorphism (2) by replying with the same tuple $\overline{a} := \overline{b}$.

In the following, we suppose that this is not the case. That is, we suppose that *the s-sphere of some of the nodes from $\overline{b}$ are different in $\mathcal{T}_{h,R}^{-k}$ and $\mathcal{T}_{h,R}$*. Observe that all nodes of $\overline{b}$ whose s-sphere is different in $\mathcal{T}_{h,R}^{-k}$ and $\mathcal{T}_{h,R}$ have to belong to the $(s-1)$-neighbourhood of the node to which $\mathcal{T}_k^0$ is attached in $\mathcal{T}_{h,R}$ but not in $\mathcal{T}_{h,R}^{-k}$, that is, the node a_{2kR}. Since the $(s-1)$-sphere of a_{2kR} is just a path of S_0-successors of length $2(s-1)$ with the centre a_{2kR} in the middle and, moreover, the nodes of $\overline{b}$ have pairwise distance $> 2s$, there is only one such node b_m, for a suitable $m \in [1, n]$. Note that the s-sphere of b_m in $\mathcal{T}_{h,R}^{-k}$ is a path of S_0-successors of length $2s$ with the centre b_m in the middle, whereas in $\mathcal{T}_{h,R}$, the s-neighbourhood of b_m also contains nodes from the substructure $\mathcal{T}_k^0$.

To find a valid reply for Duplicator, that is, a tuple $\overline{a}$ of length n of nodes from $T_{h,R}$ for which Isomorphism (2) holds, it suffices to find a node $a_m \in T_{h,R}$ that has distance $> 2s$ to each of the nodes $b_1, \ldots, b_{m-1}, b_{m+1}, \ldots, b_n$ and for which

$$\mathcal{N}_s^{\mathcal{T}_{h,R}}(a_m) \;\cong\; \mathcal{N}_s^{\mathcal{T}_{h,R}^{-k}}(b_m), \tag{3}$$

that is, the s-sphere of the node a_m in $\mathcal{T}_{h,R}$ is also a path of S_0-successors of length $2s$ with the centre a_m in the middle.

Since $n - 1 < H - 1$ and $R/2 > 2r > 2s$, we can find an $\ell \in [0, H)$ such that none of the nodes $b_1, \ldots, b_{m-1}, b_{m+1}, \ldots, b_n$ belongs to the $2s$-neighbourhood of the node $a_{2\ell R+(R/2)}$. Furthermore, by construction of $\mathcal{T}_{h,R}$, the s-sphere of $a_{2\ell R+(R/2)}$ is a path of S_0-successors of length $2s$ with the centre $a_{2\ell R+(R/2)}$ in the middle. Hence, Isomorphism (3) holds if Duplicator chooses $a_m := a_{2\ell R+(R/2)}$. Thus, Duplicator can reply with the tuple $b_1, \ldots, b_{m-1}, a_m, b_{m+1}, \ldots, b_n$ satisfying Isomorphism (2).

This completes the proof of Claim 2. In particular, Lemma 9.4.4 implies that, for each $h \geq 1$, every GNF-sentence from FO+unT$[\tau_d]$ that is $\mathfrak{T}_d$-equivalent to $\varphi_{d,h}$, has size $\geq |\mathfrak{T}_{d,2^h}|$. This concludes the proof of Lemma 9.4.9. $\square$

9.4.4 Binary Trees

This section is devoted to the proof of Theorem 9.4.2, which is implied by Corollary 9.2.10 and the following lemma.

Lemma 9.4.10. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h)_{h\geq 1}$ of sentences from $\mathsf{FO}[E]$ such that for every $h \geq 1$,*

(1) $||\varphi_h|| \leq c \cdot \mathrm{Tower}(h)$, *and*

(2) every GNF*-sentence in* $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[E]$ *that is* $\mathfrak{BT}$*-equivalent to* φ_h *has size* $\geq \mathrm{Tower}(h{+}3)$.

The proof of Lemma 9.4.10 is very similar to the proof of Lemma 9.4.9 in the previous section. The major difference is that we use the encoding of numbers by binary trees over the signature (E), introduced in the second part of Section 9.2.3, instead of ordered and labelled trees of arity 2 over the signature τ_3.

Thus, we define the sentences φ_h, $h \geq 1$, and the structures these sentences are talking about in a different way. The argumentation for showing that Duplicator has a winning strategy in the Tower(h+3)-game for φ_h on $\mathfrak{BT}$ can be taken almost verbatim from the proof of Lemma 9.4.9. In the following, we will therefore use mostly the same notation as in the proof of Lemma 9.4.9.

Proof of Lemma 9.4.10. Let $h \geq 1$ and let $H \coloneqq \mathrm{Tower}(h{+}3)$. For each $R \geq 6$, we define the following binary trees from $\mathfrak{BT}$:

- $\mathcal{C}_{h,R}$ is a path along nodes $a_0, \dots, a_{2(H+1)R}$, that is, the (E)-structure with universe $\{a_0, \dots, a_{2(H+1)R}\}$ and where for all $i, j \in [0, 2(H{+}1)R]$, the tuple (a_i, a_j) belongs to $E^{\mathcal{C}_{h,R}}$ if and only if $j = i + 1$.

- For each $i \in [0, H)$, $\mathcal{T}_i^0$ and $\mathcal{T}_i^1$ are copies of the same binary tree from $\mathfrak{B}_h(i)$, whose universe each is disjoint to the universe of $\mathcal{C}_{h,R}$. Moreover, the universes of all $\mathcal{T}_i^j$ for all $i \in [0, H)$ and $j \in \{0, 1\}$ are also pairwise disjoint.

- The binary tree $\mathcal{T}_{h,R} \in \mathfrak{BT}$ is obtained by attaching all $\mathcal{T}_i^j$ with $i \in [0, H)$ and $j \in \{0, 1\}$ to the path $\mathcal{C}_{h,R}$. More precisely, $\mathcal{T}_{h,R}$ is build from the union of $\mathcal{C}_{h,R}$ with all $\mathcal{T}_i^j$ for all $i \in [0, H)$ and $j \in \{0, 1\}$, and for each $i \in [0, H)$ and $j \in \{0, 1\}$, there is an additional edge from the node $a_{(2i+j)R}$ on the path to the root node of $\mathcal{T}_i^j$.

- For each $k \in [0, H)$, we denote by $\mathcal{T}_{h,R}^{-k}$ the substructure of $\mathcal{T}_{h,R}$ induced by removing all the nodes that belong to the universe of $\mathcal{T}_k^0$.

We will now define $\mathsf{FO}[E]$-sentences φ_h for $h \geq 1$ that have size $\mathcal{O}(\mathrm{Tower}(h))$ and for which Duplicator has a winning strategy in the H-game on $\mathfrak{BT}$. The sentences follow the same idea as the ones of Lemma 9.4.9, but are adapted to the binary trees defined above.

Claim 1. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h)_{h\geq 1}$ of sentences from $\mathsf{FO}[E]$ such that for each $h \geq 1$, $||\varphi_h|| \leq c \cdot \mathrm{Tower}(h)$, and for all $R \geq 6$,*

$$\mathcal{T}_{h,R} \models \varphi_h \quad \textit{and} \quad \mathcal{T}_{h,R}^{-k} \not\models \varphi_h \quad \textit{for all } k \in [0, H). \tag{1}$$

Proof of Claim 1. Our first task is it to find an $\mathsf{FO}[E]$-formula $\mathrm{root}(x)$ that recognises the roots of the subtrees $\mathcal{T}_i^j$ in the binary trees just defined. In the following, we call a path *branchless* if all but the first and the last of its nodes have only one child node, that is, the only child is the successor of the node on the path. Observe that none of the binary trees $\mathcal{T}_i^j$, for no $i \in [0, H)$ and $j \in \{0, 1\}$, contains a branchless path of length ≥ 5. Furthermore, the root of each such binary tree has two children. Thus, since $R \geq 6$, we can identify the root nodes of the binary tree encodings $\mathcal{T}_i^j$ in the binary trees $\mathcal{T}_{h,R}$ and $\mathcal{T}_{h,R}^{-k}$ as the nodes x with the following properties:

- The node x has two children.
- The node x is a child of a node y which is also the first node of a branchless path of length 5, which, in particular, does not contains the node x.

Thus, we can choose

$$\begin{aligned}\mathrm{root}(x) \;:=\;\; & \exists y \exists y' \big(E(x, y) \;\wedge\; E(x, y') \;\wedge\; \neg y{=}y'\big) \;\wedge \\ & \exists y \big(E(y, x) \;\wedge\; \exists y' \;\mathrm{bpath}_5(y, y')\big)\end{aligned}$$

where $\mathrm{bpath}_5(y, y')$ is an $\mathsf{FO}[E]$-formula that is satisfied if there is a branchless path of length 5 from y to y'.

Using the formulae provided by Lemma 9.2.8, we now let

$$\varphi_h \;:=\; \forall x \Big(\mathrm{root}(x) \;\rightarrow\; \exists y \left(\mathrm{root}(y) \;\wedge\; \mathrm{eq}_h(x, y) \;\wedge\; \neg x{=}y\right)\Big).$$

It is straightforward to verify that, for each $h \geq 1$, φ_h satisfies Statement (1). Furthermore, by Lemma 9.2.8, there is a number $c \in \mathbb{N}_{\geq 1}$ such that $||\varphi_h|| \leq c \cdot h$ for all $h \geq 1$. This completes the proof of Claim 1.

The following claim is proven in the same way as Claim 2 in the proof of Lemma 9.4.9, with the only modification of using the formulae φ_h just defined instead of $\varphi_{d,h}$, and the binary trees introduced above.

Claim 2. *For each $h \geq 1$, Duplicator has a winning strategy in the H-game for φ_h on $\mathfrak{BT}$.*

By Lemma 9.4.4, Claim 2 implies that for each $h \geq 1$, every GNF-sentence from $\mathsf{FO}+\mathrm{un}\mathsf{T}[E]$ that is $\mathfrak{BT}$-equivalent to φ_h, has size $\geq H = \mathrm{Tower}(h+3)$. This completes the proof of Lemma 9.4.10. □

9.4.5 Labelled Chains

This section is devoted to the proof of Theorem 9.4.3, which is implied by Corollary 9.2.2 and the following lemma.

Lemma 9.4.11. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h)_{h\geq 1}$ of sentences from $\mathsf{FO}[\tau_2]$ such that for every $h \geq 1$,*

(1) $||\varphi_h|| \leq c \cdot h$, and

(2) every GNF-sentence in $\mathsf{FO}+\mathrm{un}\mathsf{T}[\tau_2]$ that is $\mathfrak{T}_2$-equivalent to φ_h has size $\geq 2^{2^h}$.

Proof. The proof is similar to the one of Lemma 9.4.9 and Lemma 9.4.10. Instead of (binary) trees, it uses labelled chains. These labelled chains contain encodings (of the binary expansion) of natural numbers and large "gaps" inbetween. Instead of removing sub-trees (as in the proof of Lemma 9.4.9 and Lemma 9.4.10) we change the labelling of the chain to replace encodings of natural numbers by "gaps".

Let $h \geq 1$ and let $H := 2^{2^h}$. For each $i \in [0, H)$, let $w_i := v_0 \dots v_{2\cdot 2^h}$ be the bit string of length $2 \cdot 2^h + 1$ where $v_{2j} = 0$ for all $j \in [0, 2^h]$, and where $v_{2j+1} = \mathrm{bit}(j, i)$ for all $j \in [0, 2^h)$. The odd positions of w_i represent the binary expansion of the number i. Leaving the even positions labelled with 0 will allow us to mark the starting positions of the words w_i in labelled chains by words 11.

For each subset $I \subseteq [0, H)$ and every $R \geq 0$ let

$$w_R^I \;:=\; 0^{R+1}\, u_0^0\, 0^{R+1}\, u_0^1\, 0^{R+1}\, u_1^0\, 0^{R+1}\, u_1^1\, \cdots\, 0^{R+1}\, u_{H-1}^0\, 0^{R+1}\, u_{H-1}^1 \tag{1}$$

the bit string where, for each $i \in [0, H)$, $u_i^0 := 11w_i$, and where

$$u_i^1 \;:=\; \begin{cases} u_i^0 & \text{if } i \in I \text{, and} \\ 0^{|u_i^0|} & \text{if } i \notin I. \end{cases}$$

Finally, let $\mathcal{C}_{h,R}$ denote the labelled chain corresponding to the bit string $w_R^{[0,H)}$ and, for each $k \in [0, H)$, let $\mathcal{C}_{h,R}^{-k}$ denote the labelled chain corresponding to the bit string $w_R^{[0,H)\setminus\{k\}}$. Intuitively, this means that $\mathcal{C}_{h,R}$ contains two copies of each of the words w_i for all $i \in [0,H)$, each prefixed by a word of 0's of length $R+1$ and the word 11. And $\mathcal{C}_{h,R}^{-k}$ is identical two $\mathcal{C}_{h,R}$ with the only exception that one copy of the word $11w_k$ is replaced by a sequence of 0's of the same length.

Claim 1. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h)_{h\geq 1}$ of sentences from $\mathsf{FO}[\tau_2]$ such that for each $h \geq 1$, $||\varphi_h|| \leq c \cdot h$, and for all $R \geq 2$,*

$$\mathcal{C}_{h,R} \models \varphi_h \quad \textit{and} \quad \mathcal{C}_{h,R}^{-k} \not\models \varphi_h \quad \textit{for all } k \in [0,H). \tag{2}$$

Proof of Claim 1. Let $\mathcal{C}$ be one of the labelled chains $\mathcal{C}_{h,R}$ and $\mathcal{C}_{h,R}^{-k}$, $k \in [0,H)$. By construction of the bit strings defining $\mathcal{C}$, the nodes corresponding to the first position of one of the bit strings w_i, $i \in [0,H)$, are precisely the nodes which directly follow on two nodes labelled with 1. We express this observation in the formula

$$\mathrm{root}(z) \;\coloneqq\; \exists x \exists y\, (L(x) \;\wedge\; S_0(x,y) \;\wedge\; L(y) \;\wedge\; S_0(y,z)).$$

By construction of $\mathcal{C}$, for any node a of $\mathcal{C}$ that satisfies the formula $\mathrm{root}(z)$, the induced substructure $\mathcal{S}^{\mathcal{C}}_{2^{h+1}}(a)$ is a labelled chain of length 2^{h+1} and thus complete with height 2^{h+1}. Thus, the formula $\mathrm{iso}_{2,h+1}(x,x')$ of Lemma 9.2.3 is satisfied by two such nodes a, a' if and only if $\mathcal{S}^{\mathcal{C}}_{2^{h+1}}(a) \cong \mathcal{S}^{\mathcal{C}}_{2^{h+1}}(a')$.

With this observation, we can let

$$\varphi_h \;\coloneqq\; \forall x \Big(\mathrm{root}(x) \;\rightarrow\; \exists y\, (\mathrm{root}(y) \;\wedge\; \mathrm{iso}_{2,h+1}(x,y) \;\wedge\; \neg x{=}y)\Big).$$

By Lemma 9.2.3, there is a number $c \in \mathbb{N}_{\geq 1}$ such that $||\varphi_h|| \leq c \cdot h$ for all $h \geq 1$. Furthermore, it is straightforward to verify that φ_h satisfies Statement (2). This completes the proof of Claim 1.

By Lemma 9.4.4, the proof of Lemma 9.4.11 is completed by proving the following claim.

Claim 2. *For each $h \geq 1$, Duplicator has a winning strategy in the H-game for φ_h on $\mathfrak{T}_2$.*

Proof of Claim 2. Let $h \geq 1$. In the following, we describe Duplicator's winning strategy in the H-game for φ_h on $\mathfrak{T}_2$. Altogether, the winning strategy is similar to the one described in the proof of Lemma 9.4.9. However, the use of labelled chains requires some modifications.

Round (1). Suppose that Spoiler chooses the radius $r \geq 0$. For the following, let

$$R \;\coloneqq\; 4r+2.$$

By Claim 1, Duplicator can reply with the labelled chain $\mathcal{C}_{h,R}$ to win this round.

In the following, we denote by U_i^j for $i \in [0,H)$ and $j \in \{0,1\}$ the nodes that correspond to the positions of the bit string u_i^j in any of the labelled chains $\mathcal{C}_{h,R}$ and $\mathcal{C}_{h,R}^{-k}$ with $k \in [0,H)$.

Round (2). Let $\overline{a}$ be the tuple of elements from $\mathcal{C}_{h,R}$ which Spoiler chooses in this round, and let $n \in [1,H)$ be the length of this tuple. Since $\overline{a}$ has length $< H$, there has to be a $k \in [0,H)$ such that none of the nodes of $\overline{a}$ is contained in the $(R/2)$-neighbourhood of U_k^1 in $\mathcal{C}_{h,R}$.

The labelled chain $\mathcal{C}_{h,R}^{-k}$ has the same universe as $\mathcal{C}_{h,R}$ and thus still contains all the nodes of $\overline{a}$. In particular, the entire $(R/2)$-sphere of $\overline{a}$ remains unchanged. Since $R/2 > 2r$,

$$\mathcal{N}_r^{\mathcal{C}_{h,R}}(\overline{a}) \;\cong\; \mathcal{N}_r^{\mathcal{C}_{h,R}^{-k}}(\overline{a})$$

and, by Claim 1, $\mathcal{C}_{h,R}^{-k} \not\models \varphi_h$, Therefore, Duplicator wins the round by replying with the structure $\mathcal{C}_{h,R}^{-k}$ and the same tuple $\overline{a}$ which the Spoiler has chosen.

Round (3). Let $s \leq r$ be the radius chosen by Spoiler, let $\overline{b}$ be the $2s$-scattered tuple of nodes from $\mathcal{C}_{h,R}^{-k}$ chosen by Spoiler, and let $n \in [1,H)$ be the length of $\overline{b}$. Recall that Duplicator has to reply with a tuple $\overline{a}$ of length n, consisting of nodes from $\mathcal{C}_{h,R}$ such that

$$\mathcal{N}_s^{\mathcal{C}_{h,R}}(\overline{a}) \;\cong\; \mathcal{N}_s^{\mathcal{C}_{h,R}^{-k}}(\overline{b}). \tag{3}$$

Of course, each of the nodes in $\overline{b}$ also occurs in $\mathcal{C}_{h,R}$ and the pairwise distance of these nodes is the same as in $\mathcal{C}_{h,R}^{-k}$ and thus $> 2s$. If furthermore the s-spheres of all nodes in $\overline{b}$ are the same in $\mathcal{C}_{h,R}$ and $\mathcal{C}_{h,R}^{-k}$, Duplicator satisfies Isomorphism (3) by replying with the tuple $\overline{a} \coloneqq \overline{b}$.

In the following, we suppose that this is not the case. That is, we suppose that *the s-sphere of some of the nodes from $\overline{b}$ are different in $\mathcal{C}_{h,R}^{-k}$ and $\mathcal{C}_{h,R}$.* Observe that all nodes of $\overline{b}$ whose s-sphere is different in $\mathcal{C}_{h,R}^{-k}$ and $\mathcal{C}_{h,R}$ have to belong to the s-neighbourhood of the node set U_k^1. Thus, in $\mathcal{C}_{h,R}^{-k}$ the s-sphere of each of these nodes is a path of $2s+1$ nodes, labelled with 0, with its centre being the node in the middle of the path. On the other hand, in $\mathcal{C}_{h,R}$, the s-sphere of any of these nodes may contain nodes labelled with 1.

Suppose that $\overline{b} = (b_1, \dots, b_n)$. Without loss of generality, suppose furthermore that $b_1, \dots, b_m$, for a suitable $m \in [0, n]$, are precisely the elements of $\overline{b}$ that belong to the s-neighbourhood of U_k^1.

To find a valid reply for Duplicator, that is, a tuple $\overline{a}$ of elements from $\mathcal{C}_{h,R}$ with length n such that Isomorphism (3) holds, it suffices to find a $2s$-scattered tuple $(a_1, \dots, a_m)$ among the nodes of $\mathcal{C}_{h,R}$ such that

(a) $(a_1, \dots, a_m, b_{m+1}, \dots, b_n)$ is a $2s$-scattered set in $\mathcal{C}_{h,R}$ and

(b) the s-sphere of each a_i for all $i \in [1, m]$ is a path of $2s + 1$ nodes, labelled with 0, with its centre a_i being the node in the middle of the path.

In the following, let $c_1, \dots, c_{2H}$ denote the nodes of $\mathcal{C}_{h,R}$, corresponding to the middle positions of the bit strings 0^{R+1} in the bit strings described in (1). More precisely, c_i, for each $i \in [1, 2H]$, is the node of height

$$i(R + 2 \cdot 2^h + 4) + (R/2)$$

in $\mathcal{C}_{h,R}$.

Since $\overline{b}$ is of length $n < H$ and $R/2 > 2r \geq 2s$, there are pairwise distinct $\ell_1, \dots, \ell_m \in [1, 2H]$ such Condition (a) and Condition (b) hold for $a_1, \dots, a_m$ when letting $a_i \coloneqq c_{\ell_i}$ for all $i \in [1, m]$.

With this, the s-sphere of each a_i for all $i \in [1, m]$ in $\mathcal{C}_{h,R}$ is isomorphic to the s-sphere of b_i in $\mathcal{C}_{h,R}^{-k}$. Therefore, Duplicator wins Round (3) and the whole H-game for φ_h on $\mathfrak{T}_2$ by replying with the tuple $\overline{a} \coloneqq (a_1, \dots, a_m, b_{m+1}, \dots, b_n)$. This completes the proof of Claim 2.

Thus, by Lemma 9.4.4, every GNF-sentence in $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_2]$ that is $\mathfrak{T}_2$-equivalent to φ_h, for each $h \geq 1$, has size $\geq 2^{2^h}$. $\square$

9.5 Feferman-Vaught Decompositions

In this section, we show that the algorithm of Theorem 5.2.1 and thus, also the algorithms of Theorem 7.4.1 and Theorem 8.5.3 for the construction of $\oplus$-decompositions on classes of structures of bounded degree are basically worst-case optimal. The lower bounds already hold for the special case of input formulae from FO.

Recall from Section 9.2.1 that $\mathfrak{T}_d$ is the class of all labelled and ordered trees of arity $d - 1$. The main results of this section can be stated as follows:

Theorem 9.5.1. *Let $d \geq 3$ a degree bound. There is no algorithm that computes, on input of a sentence φ from $\mathsf{FO}[\tau_d]$, in time*

$$2^{d^{2^{o(||\varphi||)}}}$$

a 2-ary $\oplus$-decomposition for φ over $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_d]$ on the class $\mathfrak{T}_d$.

For the specific case of degree bound 3, we can show the following lower bound on the class $\mathfrak{BT}$ of binary trees (cf. Section 9.2.3) over the signature (E).

Theorem 9.5.2. *There is no algorithm that computes, on input of a sentence φ from $\mathsf{FO}[E]$, in time*

$$2^{2^{2^{o(||\varphi||)}}}$$

a 2-ary $\oplus$-decomposition for φ over $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[E]$ on the class $\mathfrak{BT}$.

For degree bound 2, we show the following lower bound on the class $\mathfrak{T}_2$ of labelled chains (cf. Section 9.2.2).

Theorem 9.5.3. *There is no algorithm that computes, on input of a sentence φ from $\mathsf{FO}[\tau_2]$, in time*

$$2^{2^{o(||\varphi||)}}$$

a 2-ary $\oplus$-decomposition for φ over $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_2]$ on the class $\mathfrak{T}_2$.

For the proofs of Theorem 9.5.1, Theorem 9.5.2, and Theorem 9.5.3, which can be found in Section 9.5.2, Section 9.5.3, and Section 9.5.4, respectively, we construct sequences of "small" FO-sentences over the corresponding signature for which we show lower bounds on the size of 2-ary $\oplus$-decompositions on the respective class of structures. These lower bounds are based on a generalisation of Proposition 23 in (the full version of) [GJL12], which is stated in the following section.

9.5.1 The Combinatorial Argument

In the following, we denote by $\mathcal{A} \oplus \mathcal{B}$ a disjoint sum of structures $\mathcal{A}$ and $\mathcal{B}$.

Lemma 9.5.4. *Let σ be a relational signature, let $\mathfrak{C}$ be a class of σ-structures, and let φ be an $\mathsf{FO}[\sigma_2]$-sentence. Let $H \geq 1$. Suppose that there is a subset $\mathfrak{D} \subseteq \mathfrak{C}$ of 2^H pairwise non-isomorphic structures such that for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}$,*

$$\mathcal{A} \oplus \mathcal{B} \models \varphi \quad \textit{iff} \quad \mathcal{A} = \mathcal{B}.$$

Then, every 2-ary $\oplus$-decomposition for φ over $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\sigma]$ on the class $\mathfrak{C}$ has size $\geq H$.

Proof. The lemma is proven by a counting argument. Let σ be a relational signature, let $\mathfrak{C}$ be a class of σ-structures, and let φ be an $\mathsf{FO}[\sigma_2]$-sentence. Let $H \geq 1$. Suppose that there is a subset $\mathfrak{D} \subseteq \mathfrak{C}$ of 2^H pairwise non-isomorphic structures such that for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}$,

$$\mathcal{A} \oplus \mathcal{B} \models \varphi \quad \text{iff} \quad \mathcal{A} = \mathcal{B}. \tag{1}$$

For a contradiction, assume that there is a 2-ary decomposition $\Delta \coloneqq (\beta, \Delta_1, \Delta_2)$ for φ over $\mathsf{FO{+}unT}[\sigma]$ on $\mathfrak{C}$ that has size $||\Delta|| < H$. In particular, Δ_1 and Δ_2 are finite sets of $\mathsf{FO{+}unT}[\sigma]$-sentences and β is a propositional formula using only the propositional symbols $X_{i,\delta}$ with $i \in [1,2]$ and $\delta \in \Delta_i$. Moreover, for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}$,

$$\mathcal{A} \oplus \mathcal{B} \models \varphi \quad \text{iff} \quad \mu_{\mathcal{A},\mathcal{B}} \models \beta \tag{2}$$

where $\mu_{\mathcal{A},\mathcal{B}} \colon \mathsf{PS} \to \{0,1\}$ assigns truth values to propositional symbols such that for all $\delta \in \Delta_1$,

$$\mu_{\mathcal{A},\mathcal{B}}(X_{1,\delta}) = 1 \quad \text{iff} \quad \mathcal{A} \models \delta,$$

and for all $\delta \in \Delta_2$,

$$\mu_{\mathcal{A},\mathcal{B}}(X_{2,\delta}) = 1 \quad \text{iff} \quad \mathcal{B} \models \delta,$$

and such that $\mu_{\mathcal{A},\mathcal{B}}(X) = 0$ for all $X \in \mathsf{PS}$ that do not occur in β.

From Equivalence (1) and Equivalence (2) we know that, for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}$,

$$\mu_{\mathcal{A},\mathcal{B}} \models \beta \quad \text{iff} \quad \mathcal{A} = \mathcal{B}. \tag{3}$$

Note that the number of propositional symbols occurring in β is less than H, and hence the number of distinct propositional assignments $\mu_{\mathcal{A},\mathcal{B}}$ with $\mathcal{A}, \mathcal{B} \in \mathfrak{D}$ is less than 2^H. Since $|\mathfrak{D}| = 2^H$, there exist distinct $\mathcal{A}, \mathcal{B} \in \mathfrak{D}$ such that $\mu_{\mathcal{A},\mathcal{A}} = \mu_{\mathcal{B},\mathcal{B}}$. In particular, $\mu_{\mathcal{A},\mathcal{A}}(X_{2,\delta}) = \mu_{\mathcal{B},\mathcal{B}}(X_{2,\delta})$ for all $\delta \in \Delta_2$ and thus also

$$\mu_{\mathcal{A},\mathcal{B}} \;=\; \mu_{\mathcal{A},\mathcal{A}}. \tag{4}$$

Due to Equivalence (3), we have

$$\mu_{\mathcal{A},\mathcal{A}} \models \beta. \tag{5}$$

Thus, from Equivalence (4), Statement (5), and Equivalence (2) we obtain that

$$\mathcal{A} \oplus \mathcal{B} \models \varphi.$$

This, however, is a contradiction to Equivalence (1). $\square$

In the subsequent sections, we will apply Lemma 9.5.4 to various classes of structures of bounded degree.

9.5.2 Ordered and Labelled Trees of Bounded Degree

This section is devoted to the proof of Theorem 9.5.1, which is a direct consequence of Corollary 9.2.2 and the following lemma.

Lemma 9.5.5. *Let $d \geq 3$ be a degree bound. There is a number $c_d \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_{d,h})_{h \geq 1}$ of $\mathsf{FO}[\tau_d]$-sentences such that for every $h \geq 1$,*

(1) $||\varphi_{d,h}|| \leq c_d \cdot h$, and

(2) every 2-ary $\oplus$-decomposition for $\varphi_{d,h}$ over $\mathsf{FO}+\mathrm{un}\mathsf{T}[E]$ on the class $\mathfrak{T}_d$ has size $\geq |\mathfrak{T}_{d,2^h}|$.

Proof. Let $d \geq 3$. For each $h \geq 1$, we denote by H the cardinality $|\mathfrak{T}_{d,2^h}|$ of the set $\mathfrak{T}_{d,2^h}$, and define the following $\mathfrak{T}_d$-structures:

- By $\mathcal{P}_H$, we denote a τ_d-structure with universe $\{a_0, \dots, a_{H-1}\}$ where the relation $S_0^{\mathcal{P}_H}$ describes a path along these nodes. That is, for all $i, j \in [0, H)$ we have $(a_i, a_j) \in S_0^{\mathcal{P}_H}$ if and only if $j = i + 1$, and the other successor relations $S_j^{\mathcal{P}_H}$ with $j \in [1, d-2]$ are empty.
- Let $\mathcal{T}_0, \dots, \mathcal{T}_{H-1}$ denote a sequence of structures from $\mathfrak{T}_d$ whose universe is pairwise disjoint and also disjoint to the universe of $\mathcal{P}_H$, and such that for each $\mathcal{T} \in \mathfrak{T}_{d,2^m}$ there is precisely one $i \in [0, H)$ with $\mathcal{T} \cong \mathcal{T}_i$.
- For each subset $I \subseteq [0, H)$, let $\mathcal{T}_I \in \mathfrak{T}_d$ the structure where all $\mathcal{T}_i$ with $i \in I$ are attached to the path $\mathcal{P}_H$. More precisely, $\mathcal{T}_I$ is built from the union of $\mathcal{P}_H$ with all $\mathcal{T}_i$ for all $i \in I$, and for each $i \in I$, there is an additional edge $(a_i, b) \in \mathcal{S}_1^{\mathcal{T}_I}$ from the node a_i on the path to the root node b of $\mathcal{T}_i$.

By $\mathfrak{D}_{d,h}$, we denote set of all structures $\mathcal{T}_I$ for all $I \subseteq [0, H)$. Clearly, $|\mathfrak{D}_{d,h}| = 2^H$.

Once we have proven the following claim, the proof of Lemma 9.5.5 is complete: It follows from Lemma 9.5.4 that, for each $h \geq 1$, every 2-ary $\oplus$-decomposition for the sentence $\varphi_{d,h}$ over $\mathsf{FO}+\mathrm{un}\mathsf{T}[\tau_d]$ on the class $\mathfrak{T}_d$ has size $\geq H = |\mathfrak{T}_{d,2^h}|$.

Claim 1. *There is a number $c_d \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_{d,h})_{h \geq 1}$ of sentences from $\mathsf{FO}[\tau_d]$ such that for every $h \geq 1$,*

(1) $||\varphi_{d,h}|| \leq c_d \cdot h$, and

(2) for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}_{d,h}$, $\mathcal{A} \oplus \mathcal{B} \models \varphi_{d,m}$ iff $\mathcal{A} = \mathcal{B}$.

Proof of Claim 1. Using the formulae provided by Lemma 9.2.3, we let

$$\varphi_{d,h} \;:=\; \forall x \Big(\text{complete}_{d,h}(x) \;\rightarrow\; \exists y \left(\text{complete}_{d,h}(y) \;\wedge\; \text{iso}_{d,h}(x,y) \;\wedge\; \neg x{=}y\right)\Big)$$

for each $h \geq 1$. By Lemma 9.2.3, there is a number $c_d \in \mathbb{N}_{\geq 1}$ such that for all $h \geq 1$, the sentence $\varphi_{d,h}$ has size $\leq c_d \cdot h$. Furthermore, it is straightforward to see that for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}_{d,h}$, the sentence $\varphi_{d,h}$ satisfies Condition (2) of Claim 1. This completes the proof of Claim 1 and thus, also the proof of Lemma 9.5.5. $\square$

9.5.3 Binary Trees

This section is devoted to the proof of Theorem 9.5.2. The proof is very similar to the one of Theorem 9.5.1 and a direct consequence of Corollary 9.2.10 and the following lemma.

Lemma 9.5.6. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h)_{h\geq 1}$ of sentences from $\mathsf{FO}[E]$ such that for every $h \geq 1$,*

(1) $||\varphi_h|| \leq c \cdot \text{Tower}(h)$*, and*

(2) every 2-ary $\oplus$-decomposition for φ_h over $\mathsf{FO}{+}\text{un}\mathsf{T}[E]$ on the class $\mathfrak{BT}$ has size $\geq \text{Tower}(h{+}3)$.

Proof. Let $h \geq 1$ and $H := \text{Tower}(h{+}3)$. We construct a set $\mathfrak{D}_h$ of binary trees in a similar way as the sets $\mathfrak{D}_{d,h}$ in the proof of Theorem 9.5.1. However, instead of structures from the sets $\mathfrak{T}_{d,2^h}$, we use the encoding of numbers by binary trees introduced in Section 9.2.3. To be able to identify the roots of these binary tree encodings, we have to put more distance between them. For this, we consider the following structures from $\mathfrak{BT}$:

- Let $\mathcal{P}_H$ denote graph over the signature (E) with universe $\{a_0, \ldots, a_{5H-1}\}$ and, for all $i, j \in [0, 5H)$, an edge $(a_i, a_j) \in E^{\mathcal{C}_H}$ if and only if $j = i + 1$.
- For each $i \in [0, H)$, we let $\mathcal{T}_i \in \mathfrak{B}_h(i)$ such that the universe of all $\mathcal{T}_i$, $i \in [0, H)$ is disjoint to the universe of $\mathcal{P}_H$ and, furthermore, the universes of all $\mathcal{T}_i, \mathcal{T}_j$ with $i, j \in [0, H)$ and $i \neq j$ are also pairwise disjoint.
- For each subset $I \subseteq [0, H)$, let $\mathcal{T}_I$ the binary tree where all $\mathcal{T}_i$ with $i \in I$ are attached to the path $\mathcal{P}_H$. More precisely, $\mathcal{T}_I$ is built from the union of $\mathcal{P}_H$ with all $\mathcal{T}_i$ for all $i \in I$, and for each $i \in I$, there is an additional edge $(a_{5i}, b) \in E^{\mathcal{T}_I}$ from the node a_i on the path to the root node b of $\mathcal{T}_i$.

By $\mathfrak{D}_h$ we denote the set of all structures $\mathcal{T}_I$ for all $I \subseteq [0, H)$. Clearly $|\mathfrak{D}_h| = 2^H$.

Once we have proven the following claim, the proof of Lemma 9.5.6 is complete: It follows from Lemma 9.5.4 that, for each $h \geq 1$, every 2-ary $\oplus$-decomposition for φ_h over $\mathsf{FO}+\mathrm{un}\mathsf{T}[E]$ on the class $\mathfrak{BT}$ has size $\geq H = \mathrm{Tower}(h+3)$.

Claim 1. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h)_{h\geq 1}$ of sentences from $\mathsf{FO}[E]$ such that for every $h \geq 1$,*

(1) $||\varphi_h|| \leq c \cdot \mathrm{Tower}(h)$, and

(2) for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}_h$, $\mathcal{A} \oplus \mathcal{B} \models \varphi_h$ iff $\mathcal{A} = \mathcal{B}$.

Proof of Claim 1. Let $h \geq 1$. For the construction of the sentence φ_h, we first have to identify the roots of the subtrees $\mathcal{T}_i$ for all $i \in [0, H)$ in the structures of $\mathfrak{D}_h$. For this, we can proceed as in the proof of Claim 1 in the proof of Lemma 9.4.10.

None of the binary trees $\mathcal{T}_i$, for no $i \in [0, H)$, contains a branchless path of length ≥ 5. Recall that a path is called branchless if all but the first and the last of its nodes have only one child. Furthermore, the root of each such binary tree has two children. Using these observations, we can see that in the binary trees in $\mathfrak{D}_h$, the subtrees $\mathcal{T}_i$, $i \in [0, H)$ are so far away from each other on the path $\mathcal{P}_H$, that their root nodes can be identified as the nodes x with the following properties:

- There is a node y with two children; one of these children being x.
- The node y is the first node of a branchless path of length 5, which does not contains x.
- The node x has two children.

Thus, we can choose

$$\begin{aligned} \mathrm{root}(x) \;:=\; & \exists y \exists y' \big(E(x, y) \;\wedge\; E(x, y') \;\wedge\; \neg y{=}y'\big) \;\wedge \\ & \exists y \big(E(y, x) \;\wedge\; \exists y' \; \mathrm{bpath}_5(y, y')\big) \end{aligned}$$

where $\mathrm{bpath}_5(y, y')$ is an $\mathsf{FO}[E]$-formula that is satisfied if there is a branchless path of length 5 from y to y'.

Using the formulae provided by Lemma 9.2.8, we now define

$$\varphi_h \;:=\; \forall x \Big(\mathrm{root}(x) \;\to\; \exists y \left(\mathrm{root}(y) \;\wedge\; \mathrm{eq}_h(x, y) \;\wedge\; \neg x{=}y\right)\Big).$$

By Lemma 9.2.8, there is a number $c \in \mathbb{N}_{\geq 1}$ such that $||\varphi_h|| \leq c \cdot \mathrm{Tower}(h)$ for each $h \geq 1$. Furthermore, it is straightforward to see that for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}_h$, the sentence φ_h satisfies Condition (2) of Claim 1. This completes the proof of Claim 1 and thus, also the proof of Lemma 9.5.6. □

9.5.4 Labelled Chains

The overall structure of the proof of Theorem 9.5.3 is the same as for Theorem 9.5.1. Using Lemma 9.1.1, Theorem 9.5.3 is implied by the following lemma.

Lemma 9.5.7. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h)_{h \geq 1}$ of sentences from $\mathsf{FO}[\tau_2]$ such that for every $h \geq 1$,*

(1) $||\varphi_h|| \leq c \cdot h$, and

(2) every 2-ary $\oplus$-decomposition for φ_h over $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_2]$ on the class $\mathfrak{T}_2$ has size $\geq 2^{2^h}$.

Proof. Let $m \geq 1$ and let $H := 2^{2^h}$. We employ a similar encoding of numbers from $[0, H)$ by labelled chains as in the proof of Lemma 9.4.11. For each $i \in [0, H)$, let w_i be the bit string of length $2^{h+1} + 1 = 2 \cdot 2^h + 1$ where precisely the positions $2j + 1$ for all $j \in [0, 2^h)$ with $\mathrm{bit}(j, i) = 1$ are labelled with 1, and all other positions are labelled with 0. Intuitively, the odd positions of the word w_i represent the binary expansion of the number i. For example, for $h = 1$ and $i = 3$, $w_i = 01010$. Note that, in particular, the last position of each word w_i is always labelled with 0.

For all $I \subseteq [0, H)$, we now denote by w_I the bit string

$$w_I \quad := \quad v_0 w_0 v_1 w_1 \cdots v_{H-1} w_{H-1},$$

where $w_0, \ldots, w_{H-1}$ are defined as above, and where $v_i = 11$ for all $i \in I$ and $v_i = 00$ for all $i \in [0, H)$ with $i \notin I$. By $\mathcal{C}_I$ we denote the labelled chain corresponding to the word w_I. Thus, each $\mathcal{C}_I$ contains the binary expansions of all numbers $i \in [0, H)$, but only the binary expansions of numbers $i \in I$ are marked by the prefix 11. Finally, let $\mathfrak{D}_h$ be the set of all labelled chains $\mathcal{C}_I$ for all $I \subseteq [0, H)$.

The proof of Lemma 9.5.7 is complete once we have proven the following claim. By Lemma 9.5.4 for each $h \geq 1$, every 2-ary decomposition for φ_h over $\mathsf{FO}{+}\mathrm{un}\mathsf{T}[\tau_2]$ on the class $\mathfrak{T}_2$ of labelled chains has size $\geq H = 2^{2^h}$.

Claim 1. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h)_{h\geq 1}$ of sentences from* $\mathsf{FO}[\tau_2]$ *such that for every $h \geq 1$,*

(1) $||\varphi_h|| \leq c \cdot h$*, and*

(2) for all $\mathcal{A}, \mathcal{B} \in \mathfrak{D}_h$, $\mathcal{A} \oplus \mathcal{B} \models \varphi_h$ *iff* $\mathcal{A} = \mathcal{B}$.

Proof of Claim 1. Note that in any labelled chain $\mathcal{C}_I$ from $\mathfrak{D}_h$, the nodes corresponding to the initial positions of the words w_i, $i \in I$, can be recognised by the formula

$$\mathrm{root}(z) \;\coloneqq\; \exists x \exists y (S_0(x,y) \;\wedge\; S_0(y,z) \;\wedge\; L(x) \;\wedge\; L(y)).$$

Using the formulae provided by Lemma 9.2.3, we let

$$\varphi_h \;\coloneqq\; \forall x \Big(\mathrm{root}(x) \;\rightarrow\; \exists y \left(\mathrm{root}(y) \;\wedge\; \mathrm{iso}_{2,h+1}(x,y) \;\wedge\; \neg x{=}y\right)\Big).$$

From Lemma 9.2.3 we know that there is a number $c \in \mathbb{N}_{\geq 1}$ such that $||\varphi_h|| \leq c \cdot h$ for all $h \geq 1$. Furthermore, it is straightforward to see that for all $\mathcal{C}_I, \mathcal{C}_J \in \mathfrak{D}_h$, the sentence φ_h is satisfied by $\mathcal{C}_I \oplus \mathcal{C}_J$ if and only if $\mathcal{C}_I = \mathcal{C}_J$ (that is, $I = J$). This completes the proof of Claim 1 and also the proof of Lemma 9.5.7. $\square$

9.6 Preservation Theorems

In this section, we provide 3-fold exponential lower bounds for our algorithms from Theorem 6.1.7 and Theorem 6.1.10. Recall that, for $d \geq 3$, Theorem 6.1.7 provided a 5-fold exponential upper bound on the construction of existential formulae for formulae from FO+unM that are preserved under extensions on the class of d-bounded structures. Similarly, Theorem 6.1.10 implied a 4-fold exponential upper bound on the construction of existential-formulae for formulae from FO+unM that are preserved under homomorphisms on the class of d-bounded structures.

Both lower bounds already hold for sentences from FO. For the lower bound concerning preservation under extensions, we let $\sigma_{\text{ext}} \coloneqq (S_0, S_1, L_0, L_1)$ be the relational signature with the binary relation symbols S_0, S_1, and the unary relation symbols L_0, L_1. Furthermore, we let $\mathfrak{C}_{\text{ext}}$ denote the class of all forest-like structures (cf. Section 9.2) over the signature σ_{ext}. Clearly, $\mathfrak{C}_{\text{ext}}$ is closed under disjoint unions and induced substructures, and all structures in $\mathfrak{C}_{\text{ext}}$ have degree at most 3.

Theorem 9.6.1. *There is no algorithm which, on input of an* $\mathsf{FO}[\sigma_{\text{ext}}]$*-sentence* φ *that is preserved under extensions on* $\mathfrak{C}_{\text{ext}}$*, computes in time*

$$2^{2^{2^{o(||\varphi||)}}}$$

an existential sentence from $\mathsf{FO}[\sigma_{\text{ext}}]$ *that is equivalent to* φ *on* $\mathfrak{C}_{\text{ext}}$*.*

For the lower bound concerning preservation under homomorphisms, we let $\sigma_{\text{hom}} \coloneqq (S_0, S_1, L_\emptyset, L_{\{0\}}, L_{\{1\}}, L_{\{0,1\}})$ be the relational signature with the binary relation symbols S_0, S_1, and, for each $M \subseteq \{0,1\}$, a unary relation symbol L_M. Furthermore, we let $\mathfrak{C}_{\text{hom}}$ denote the class of all forest-like structures $\mathcal{F}$ over the signature τ with the additional condition, that *each node of* $\mathcal{F}$ *belongs to precisely one of the unary relations* L_M *for* $M \subseteq \{0,1\}$. Also $\mathfrak{C}_{\text{hom}}$ is closed under disjoint unions and induced substructures, and all structures in $\mathfrak{C}_{\text{hom}}$ have degree at most 3.

Theorem 9.6.2. *There is no algorithm which, on input of an* $\mathsf{FO}[\sigma_{\text{hom}}]$*-sentence* φ *that is preserved under homomorphisms on* $\mathfrak{C}_{\text{hom}}$*, computes in time*

$$2^{2^{2^{o(||\varphi||)}}}$$

an existential-positive sentence from $\mathsf{FO}[\sigma_{\text{hom}}]$ *that is equivalent to* φ *on* $\mathfrak{C}_{\text{hom}}$*.*

In the following, we call a structure in one of the classes $\mathfrak{C}_{\text{ext}}$ and $\mathfrak{C}_{\text{hom}}$ an *ordered forest* and, in particular, an *ordered tree* if it is connected.

The proofs of Theorem 9.6.1 and Theorem 9.6.2 can be found in Section 9.6.2 and Section 9.6.3, respectively. They rely on the following observation, which shows that, in respect to a class of structures that is closed under induced substructures, a lower bound on the size of minimal models of a sentence is also a lower bound on the size of an equivalent existential sentence. The same holds for existential-positive sentences, since every existential-positive sentence is also an existential sentence.

Lemma 9.6.3. *Let* σ *be a relational signature and let* $\mathfrak{C}$ *be a class of* σ*-structures that is closed under induced substructures. For each* $\mathsf{FO}[\sigma]$*-sentence* φ *and every* $N \geq 1$ *the following holds:*

If φ *has a* $\mathfrak{C}$*-minimal model of size at least* N*, then every existential* $\mathsf{FO}[\sigma]$*-sentence that is* $\mathfrak{C}$*-equivalent to* φ *has size* $> N$*.*

Proof. Let σ be a relational signature and let $\mathfrak{C}$ be a class of σ-structures that is closed under induced substructures. Let φ be an $\mathsf{FO}[\sigma]$-sentence and suppose that every $\mathfrak{C}$-minimal model of φ has at least $N \geq 1$ elements.

For a contradiction, assume that ψ is an existential $\mathsf{FO}[\sigma]$-sentence of size $\leq N$ that is $\mathfrak{C}$-equivalent to φ. In particular, ψ has the shape $\exists x_1 \dots x_k \, \gamma(x_1, \dots, x_k)$ for a $k < N$ and a quantifier-free subformula $\gamma(x_1, \dots, x_k)$.

Since φ and ψ are $\mathfrak{C}$-equivalent, $\mathcal{A}$ is also a model of ψ. Thus, there are elements $a_1, \dots, a_k \in A$ such that $\mathcal{A} \models \gamma[a_1, \dots, a_k]$. As $\gamma(x_1, \dots, x_k)$ is quantifier-free, this implies that for the substructure $\mathcal{B} \coloneqq \mathcal{A}[\{a_1, \dots, a_k\}]$ of $\mathcal{A}$, induced by the elements $a_1, \dots, a_k$, also $\mathcal{B} \models \gamma[a_1, \dots, a_k]$. Thus, $\mathcal{B} \models \psi$.

Since $\mathfrak{C}$ is closed under induced substructures, also $\mathcal{B} \in \mathfrak{C}$. Furthermore, since φ and ψ are assumed to be $\mathfrak{C}$-equivalent, $\mathcal{B} \models \varphi$. However, this contradictions the assumption that $\mathcal{A}$ is a $\mathfrak{C}$-*minimal* model of φ. $\square$

To obtain sequences of slow-growing sentences with large minimal models, we use the encoding of numbers by binary trees, introduced in Section 9.2.3, and formulae expressing arithmetic over these binary trees. The latter formulae are inspired by the ones defined in [DGKS07] for tree encodings, and will be provided in Section 9.6.1.

The main challenge is to find sequences of sentences that not only have large minimal models but are also preserved under extensions or homomorphisms, respectively. To this aim, the auxiliary unary relation symbols in the signatures σ_{ext} and σ_{hom} are introduced to interpret binary tree encodings in complete[3] ordered trees from $\mathfrak{C}_{\text{ext}}$ and $\mathfrak{C}_{\text{hom}}$, respectively.

9.6.1 Arithmetic over Binary Tree Encodings

Recall that, in Lemma 9.2.8, we already constructed formulae $\text{eq}_h(x, y)$ which, for each $h \geq 1$, were able to recognise binary tree encodings that encode the same number $< \text{Tower}(h{+}3)$ by analysing the subtrees below the root nodes x and y. The formulae $\text{eq}_h(x, y)$ were obtained by adapting similar formulae for tree encodings (of arbitrary degree) as presented in Lemma 3.2 of [DGKS07] and Lemma 10.21 of [FG06]. Lemma 3.3 and Lemma 3.4 of [DGKS07] define arithmetic relations between tree encodings. Aim of this section is to also adapt these to binary tree encodings.

[3] Note that, since the structures in the classes $\mathfrak{C}_{\text{ext}}$ and $\mathfrak{C}_{\text{hom}}$ are forest-like, we can use the notation introduced in Section 9.2.

After this is done, we use the constructed formulae to obtain a sequence $(\varphi_h)_{h\geq 1}$ of $\mathsf{FO}[E]$-sentences of size $\mathcal{O}(\mathrm{Tower}(h))$ where, for each $h \geq 1$, the sentence φ_h has a $\mathfrak{BF}$-minimal model with a universe of size $> \mathrm{Tower}(h{+}3)$. However, it will require more work to modify these sentences such that they are also preserved under extensions or homomorphisms, respectively, on $\mathfrak{BF}$.

Lemma 9.6.4. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\mathrm{enc}_h(x))_{h\geq -1}$ of $\mathsf{FO}[E]$-sentences of size $\leq c \cdot \mathrm{Tower}(h)$, for $h \geq 0$, such that for each $h \geq -1$ the following holds:*

If $\mathcal{F}$ is a binary forest from $\mathfrak{BF}$ and $a \in F$, then

$$\mathcal{F} \ \models \ \mathrm{enc}_h[a] \quad \textit{iff} \quad \mathcal{S}^{\mathcal{F}}(a) \in \mathfrak{B}_h(i) \textit{ for an } i \in [0, \mathrm{Tower}(h{+}3)).$$

Recall the formulae $\mathrm{path}_{\leq n}(x,y)$ of size $\mathcal{O}(\log n)$, for $n \geq 1$, given by Lemma 2.7.1, that are satisfied by nodes a, b of a binary forest $\mathcal{F}$ if there is a path of length $\leq n$ from a to b in $\mathcal{F}$. In the following, we furthermore let

$$\mathrm{path}_{=n}(x,y) \ :=\ \ \mathrm{path}_{\leq n}(x,y) \ \wedge\ \neg\, \mathrm{path}_{\leq n-1}(x,y)$$

the formula of size $\mathcal{O}(\log n)$ that is satisfied by a and b if there is a path of length *precisely* n from a to b in $\mathcal{F}$.

Proof of Lemma 9.6.4. For $h = -1$, recall that, by Definition 9.2.7, the set $\mathfrak{B}_{-1}(i)$ of binary tree encodings of i with parameter -1 is only defined for the numbers $i \in \{0,1,2,3\}$, and for each of these numbers, $\mathfrak{B}_{-1}(i)$ contains all binary trees that are isomorphic to the tree encoding $\mathcal{T}(i)$ depicted in Figure 9.1.

For each such $i \in \{0,1,2,3\}$, it is straightforward to construct a formula $\mathrm{enc}_{-1,i}(x)$ from $\mathsf{FO}[E]$ that is satisfied in a binary forest if x is the root of a subtree isomorphic to $\mathcal{T}(i)$. The formula $\mathrm{enc}_{-1}(x)$ can then be chosen as the disjunction of all formulae $\mathrm{enc}_{-1,i}(x)$ for all $i \in \{0,1,2,3\}$.

Let $h \geq 0$. By Definition 9.2.7, we have to define the $\mathsf{FO}[E]$-formula $\mathrm{enc}_h(x)$ such that it is satisfied by a node a in a binary forest $\mathcal{F}$ if and only if

(1) the subtree $\mathcal{S}^{\mathcal{F}}_{\mathrm{Tower}(h+1)-1}(a)$ is complete with height $\mathrm{Tower}(h{+}1) - 1$, and

(2) for every node b that can be reached from a by a path of length $\mathrm{Tower}(h{+}1)$, $\mathcal{S}^{\mathcal{F}}(b) \in \mathfrak{B}_{h-1}(j)$ for some $j \in [0, \mathrm{Tower}(h{+}2))$.

With the same idea as in the proof of Lemma 9.2.3, we can define a formula that recognises nodes a of binary forests $\mathcal{F}$, where the subtree induced by all nodes reachable from a by a path of length $\leq n$ is a complete binary tree of height n. For each $n \geq 1$, let

$$\begin{aligned} \text{complete}_n(x) \ :=\ & \exists y\ \text{path}_{=n}(x,y)\ \wedge \\ & \forall y\ \Big(\text{path}_{\leq n-1}(x,y)\ \rightarrow \\ & \qquad \exists z_0 \exists z_1\ \big(E(y,z_0)\ \wedge\ E(y,z_1)\ \wedge\ \neg z_0{=}z_1\big)\Big). \end{aligned}$$

The formula states that there is a node y that is reachable from x by a path of length precisely n, and that every other node y that is reachable from x by a path of length $< n$ has exactly two children. Thus, in each binary forest $\mathcal{F}$ and for every $a \in F$, $\mathcal{F} \models \text{complete}_n[a]$ if and only if $\mathcal{S}_n^{\mathcal{F}}(a)$ is a complete binary tree of height n. Observe that also $\text{complete}_n(x)$ has size in $\mathcal{O}(\log n)$.

Using this formula, we can define $\text{enc}_h(x)$ recursively by choosing

$$\begin{aligned} \text{enc}_h(x)\ :=\ & \text{complete}_{\text{Tower}(h+1)-1}(x)\ \wedge \\ & \forall y\ \big(\text{path}_{=\text{Tower}(h+1)}(x,y)\ \rightarrow\ \text{enc}_{h-1}(y)\big). \end{aligned}$$

In the latter formula, the first line verifies Condition (1) while the second line verifies Condition (2).

Observe that the formulae $\text{complete}_{\text{Tower}(h+1)-1}(x)$ and $\text{path}_{=\text{Tower}(h+1)}$ have size in $\mathcal{O}(\text{Tower}(h))$ for $h \geq 0$. Thus, Observation 9.2.9 implies that there is a number $c \in \mathbb{N}_{\geq 1}$ such that for all $h \geq 0$, we have $||\,\text{enc}_h\,|| \leq c \cdot \text{Tower}(h)$. This completes the proof of Lemma 9.6.4. $\square$

Lemma 9.6.5. *There is a number* $c \in \mathbb{N}_{\geq 1}$ *and sequences* $(\min_h(x))_{h\geq -1}$, $(\text{less}_h(x,y))_{h\geq -1}$, $(\text{succ}_h(x,y))_{h\geq -1}$, *and* $(\max_h(x))_{h\geq -1}$ *of formulae from* $\mathsf{FO}[E]$ *of size* $\leq c \cdot \text{Tower}(h)$, *for* $h \geq 0$, *such that for each* $h \geq -1$ *the following holds:*

If $\mathcal{F}$ *is a binary forest from* $\mathfrak{BF}$ *and* $a, b \in F$ *such that there are numbers* $i, j \in [0, \text{Tower}(h{+}3))$ *with* $\mathcal{S}^{\mathcal{F}}(a) \in \mathfrak{B}_h(i)$ *and* $\mathcal{S}^{\mathcal{F}}(b) \in \mathfrak{B}_h(j)$, *then*

$$\begin{array}{lllll} \mathcal{F} & \models & \min_h[a] & \textit{iff} & i = 0, \\ \mathcal{F} & \models & \text{less}_h[a,b] & \textit{iff} & i < j, \\ \mathcal{F} & \models & \text{succ}_h[a,b] & \textit{iff} & i + 1 = j, \quad \textit{and} \\ \mathcal{F} & \models & \max_h[a] & \textit{iff} & i = \text{Tower}(h{+}3) - 1. \end{array}$$

Proof. For $h = -1$, the formulae can be straightforwardly defined using the formulae $\text{enc}_{-1,i}(x)$ for $i \in \{0,1,2,3\}$, introduced in the proof of Lemma 9.6.4. More precisely, we choose $\min_{-1}(x) := \text{enc}_{-1,0}(x)$ and $\max_{-1}(x) := \text{enc}_{-1,3}(x)$. Furthermore, we let $\text{less}_{-1}(x,y)$ the disjunction over all $\text{enc}_{-1,i}(x) \wedge \text{enc}_{-1,j}(x)$

with $i, j \in \{0, 1, 2, 3\}$ such that $i < j$, and we let $\mathrm{succ}_{-1}(x, y)$ the disjunction over all $\mathrm{enc}_{-1,i}(x) \wedge \mathrm{enc}_{-1,i+1}(x)$ for $i \in \{0, 1, 2\}$.

Let $h \geq 0$. In this case, the construction of the formulae $\min_h(x)$, $\mathrm{less}_h(x, y)$, $\mathrm{succ}_h(x, y)$, and $\max_h(x)$ is based on the binary expansion of numbers satisfying the respective arithmetic relation. To access the bits of the binary expansion of the number encoded by a binary tree, we abbreviate in the following

$$\pi_h(x, y) \quad := \quad \mathrm{path}_{=\mathrm{Tower}(h+1)}(x, y).$$

Observe that the formula $\pi_h(x, y)$ has size in $\mathcal{O}(\mathrm{Tower}(h))$ for $h \geq 0$.

For the formula $\min_h(x)$, observe that no bit is set in the binary expansion of the number 0. Thus, we can choose

$$\min_h(x) \quad := \quad \neg\exists y\, \pi_h(x, y),$$

which has also size in $\mathcal{O}(\mathrm{Tower}(h))$.

For the formula $\mathrm{less}_h(x, y)$, observe that in the binary expansions of numbers i and j with $i < j$, there is a bit which is set in the binary expansion of j but not in i, and every higher valued bit that is set in the binary expansion of i is also set in the binary expansion of j. Thus, we can choose

$$\begin{aligned} \mathrm{less}_h(x, y) \quad := \quad \exists y' \Big(\pi_h(y, y') \wedge \\ & \forall x' \left(\pi_h(x, x') \;\rightarrow\; \neg\, \mathrm{eq}_{h-1}(x', y')\right) \wedge \\ & \forall x'' \left((\pi_h(x, x'') \;\wedge\; \mathrm{less}_{h-1}(y', x''))\right. \\ & \qquad \left.\rightarrow\; \exists y'' \left(\pi_h(y, y'') \;\wedge\; \mathrm{eq}_{h-1}(y'', x'')\right)\right)\Big). \end{aligned}$$

Recall that the formulae $\pi_h(x, y)$ and $\mathrm{eq}_{h-1}(x, y)$ have size in $\mathcal{O}(\mathrm{Tower}(h))$ and in $\mathcal{O}(\mathrm{Tower}(h-1))$, respectively, and that $\mathrm{less}_h(x, y)$ has only one recursive call of $\mathrm{less}_{h-1}(x, y)$. Thus, we can conclude from Observation 9.2.9 that less_h has size in $\mathcal{O}(\mathrm{Tower}(h))$.

For the formula $\mathrm{succ}_h(x, y)$, we can proceed in a similar way as for the formula

$\mathrm{less}_h(x, y)$. That is, we let

$$
\begin{aligned}
\mathrm{succ}_h(x, y) \ \coloneqq \quad & \exists y' \Big(\pi_h(y, y') \\
& \wedge \ \ \forall y'' \left((\pi_h(y, y'') \ \wedge \ \neg\, \mathrm{eq}_{h-1}(y'', y')) \ \rightarrow \ \mathrm{less}_{h-1}(y', y'') \right) \\
& \wedge \ \ \forall x' \left(\pi_h(x, x') \ \rightarrow \ \neg\, \mathrm{eq}_{h-1}(x', y') \right) \\
& \wedge \ \ \forall y'' \left((\pi_h(y, y'') \ \wedge \ \mathrm{less}_{h-1}(y', y'')) \right. \\
& \qquad\qquad \left. \rightarrow \ \exists x'' \left(\pi_h(x, x'') \ \wedge \ \mathrm{eq}_{h-1}(x'', y'') \right) \right) \\
& \wedge \ \ \forall x'' \left((\pi_h(x, x'') \ \wedge \ \mathrm{less}_{h-1}(y', x'')) \right. \\
& \qquad\qquad \left. \rightarrow \ \exists y'' \left(\pi_h(y, y'') \ \wedge \ \mathrm{eq}_{h-1}(y'', x'') \right) \right) \\
& \wedge \ \ \Big(\neg\, \mathrm{min}_{h-1}(y') \\
& \qquad \rightarrow \ \big(\exists x' \left(\pi_h(x, x') \ \wedge \ \mathrm{min}_{h-1}(x') \right) \\
& \qquad\qquad \wedge \ \forall x' \left((\pi_h(x, x') \ \wedge \ \mathrm{less}_{h-1}(x', y')) \right. \\
& \qquad\qquad\qquad \rightarrow \ \exists z \left(\mathrm{succ}_{h-1}(x', z) \right. \\
& \qquad\qquad\qquad\qquad \left.\left. \wedge \ (z{=}y' \ \vee \ \pi_h(x, z)) \right) \right) \big) \Big) \Big).
\end{aligned}
$$

Since the subformulae $\mathrm{less}_{h-1}(x, y)$, $\mathrm{eq}_{h-1}(x, y)$, and $\mathrm{min}_{h-1}(x)$ have size in $\mathcal{O}(\mathrm{Tower}(h{-}1))$ and $\mathrm{succ}_h(x, y)$ furthermore uses only one recursive call of $\mathrm{succ}_{h-1}(x, y)$, Observation 9.2.9 implies that $\mathrm{succ}_h(x, y)$ has size in $\mathcal{O}(\mathrm{Tower}(h))$.

For the formula $\mathrm{max}_h(x)$, we finally let

$$
\begin{aligned}
\mathrm{max}_h(x) \ \coloneqq \quad & \exists y \left(\pi_h(x, y) \ \wedge \ \mathrm{min}_{h-1}(y) \right) \ \wedge \\
& \forall y \left(\pi_h(x, y) \right. \\
& \qquad \left. \rightarrow \ \left(\mathrm{max}_{h-1}(y) \ \vee \ \exists z \left(\pi_h(x, z) \ \wedge \ \mathrm{succ}_{h-1}(y, z) \right) \right) \right).
\end{aligned}
$$

Again, Observation 9.2.9 leads to the conclusion that $\mathrm{max}_h(x)$ has size in $\mathcal{O}(\mathrm{Tower}(h))$.

Altogether there is a number $c \in \mathbb{N}_{\geq 1}$ such that for each $h \geq 0$, the formulae $\mathrm{min}_h(x)$, $\mathrm{less}_h(x, y)$, $\mathrm{succ}_h(x, y)$, and $\mathrm{max}_h(x)$ have size $\leq c \cdot \mathrm{Tower}(h)$. This completes the proof of Lemma 9.6.5. □

With the $\mathsf{FO}[E]$-formulae defined in Lemma 9.6.4 and Lemma 9.6.5, a sequence $(\varphi_h)_{h\geq 1}$ of $\mathsf{FO}[E]$-sentences with large $\mathfrak{BF}$-minimal models can be defined by choosing, for each $h \geq 1$,

$$\begin{aligned}\varphi_h \;:=\;\; & \exists x \, (\mathrm{enc}_h(x) \;\wedge\; \min_h(x)) \;\wedge \\ & \forall x \left(\mathrm{enc}_h(x) \;\rightarrow\; \Big(\max_h(x) \;\vee\; \exists y \, (\mathrm{enc}_h(y) \;\wedge\; \mathrm{succ}_h(x,y)) \Big) \right). \end{aligned} \tag{9.1}$$

By the definitions of the subformulae in Lemma 9.6.4 and Lemma 9.6.5, the sentences φ_h have clearly size in $\mathcal{O}(\mathrm{Tower}(h))$. For each $h \geq 1$, the sentence φ_h expresses in a binary forest that there is a node which is the root of a binary tree encoding of the number 0, and for each root node of a binary tree encoding of a number $i < \mathrm{Tower}(h{+}3) - 1$, there exists another node which is the root of a binary tree encoding of $i + 1$. Thus, every model of φ_h contains binary tree encodings (with parameter h) of each number $i \in [0, \mathrm{Tower}(h{+}3))$ and thus, has more than $\mathrm{Tower}(h{+}3)$ elements.

On the other hand, already the trees depicted in Figure 9.1 illustrate that φ_h is not preserved under extensions since an extension of a model of φ_h may change the numbers encoded in the binary tree encodings of the model.

In the proofs of Theorem 9.6.1 and Theorem 9.6.2 in the subsequent sections, we will solve this problem by embedding binary tree encodings in complete ordered binary forests of suitable height over the signatures σ_{ext} and σ_{hom}, respectively. This is done in such a way that no extension and no homomorphic image, respectively, changes the embedded binary tree encoding.

To this aim, the following observation about the height of binary tree encodings will be important.

Lemma 9.6.6. *For each $h > 1$ and every $i \in [0, \mathrm{Tower}(h{+}3))$, each binary tree in $\mathfrak{B}_h(i)$ has height $< 2 \cdot \mathrm{Tower}(h{+}1)$.*

Proof. Every binary tree encoding in $\mathfrak{B}_{-1}(i)$ for all $i \in \{0, 1, 2, 3\}$ has height at most 2. For $h \geq 0$, it follows from Definition 9.2.7 that each binary tree in $\mathfrak{B}_h(i)$ for all $i \in [0, \mathrm{Tower}(h{+}3))$ has height at most

$$2 + \sum_{k=0}^{h} \mathrm{Tower}(k{+}1).$$

By a straightforward induction it can be shown that, for all $h > 1$, the latter value is $< 2 \cdot \mathrm{Tower}(h{+}1)$. $\square$

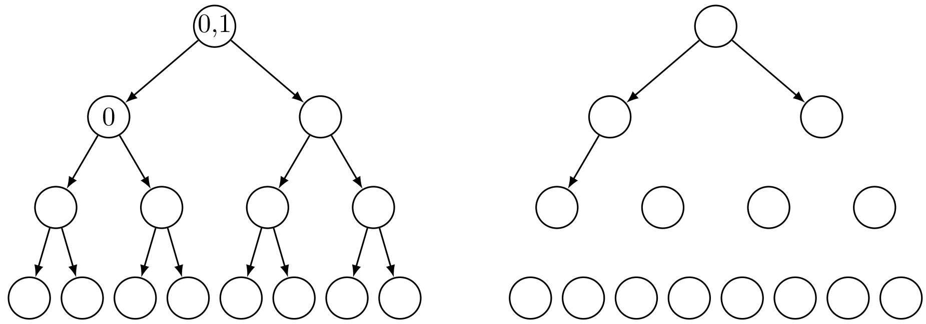

Figure 9.4 On the left side, a complete ordered binary tree $\mathcal{A} \in \mathfrak{C}_{\text{ext}}$ of height 3 is shown. Here, a node is labelled with 0 if it is contained in the relation $L_0^{\mathcal{A}}$, and it is labelled with 1 if it is contained in the relation $L_1^{\mathcal{A}}$. Recall that the edges of this tree are ordered. That is, the edges directed to the left belong to the relation $S_0^{\mathcal{A}}$ while the edges directed to the right belong to the relation $S_1^{\mathcal{A}}$. The forest on the right is the *unordered* binary forest $\Theta^{\text{ext}}[\mathcal{A}]$ of height 2 from $\mathfrak{BF}$, embedded in $\mathcal{A}$.

9.6.2 Preservation under Extensions

This section is devoted to the proof of Theorem 9.6.1. Recall the signature $\sigma_{\text{ext}} = (S_0, S_1, L_0, L_1)$ with the binary relations S_0 and S_1, and the unary relations L_0 and L_1. We embed binary forests from $\mathfrak{BF}$, that is, over the signature (E), in complete ordered binary trees from $\mathfrak{C}_{\text{ext}}$ over the signature σ_{ext}.

This will be described by a transduction $\Theta^{\text{ext}} := (\theta^{\text{ext}}, \theta_E^{\text{ext}})$ from σ_{ext} to (E), defined by $\theta^{\text{ext}}(x) := x{=}x$ and

$$\theta_E^{\text{ext}}(x,y) \;:=\; \big(S_0(x,y) \wedge L_0(x)\big) \vee \big(S_1(x,y) \wedge L_1(x)\big).$$

Observe that for every ordered binary forest $\mathcal{A}$ from $\mathfrak{C}_{\text{ext}}$, $\Theta^{\text{ext}}[\mathcal{A}]$ is the unordered binary forest from $\mathfrak{BF}$ over the signature (E), which contains the same nodes as $\mathcal{A}$ and for all nodes $a, b \in A$, there is an edge from a to b in $\Theta^{\text{ext}}[\mathcal{A}]$ if $(a,b) \in S_0^{\mathcal{A}}$ and $a \in L_0^{\mathcal{A}}$, or if $(a,b) \in S_1^{\mathcal{A}}$ and $a \in L_1^{\mathcal{A}}$. Intuitively, the unary relation $L_0^{\mathcal{A}}$ indicates whether an edge from a to a node b in $S_0^{\mathcal{A}}$ is an edge in $\Theta[\mathcal{A}]$, too, and analogous for $L_1^{\mathcal{A}}$ and $S_1^{\mathcal{A}}$. See Figure 9.4 for an illustration.

Theorem 9.6.1 follows directly from Corollary 9.2.10 and the following lemma.

Lemma 9.6.7. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h^{\text{ext}})_{h>1}$ of sentences from $\mathsf{FO}[\sigma_{\text{ext}}]$ such that for each $h > 1$,*

(1) $||\varphi_h^{\text{ext}}|| \leq c \cdot \text{Tower}(h)$,

(2) every existential $\mathsf{FO}[\sigma_{\text{ext}}]$*-sentence that is* $\mathfrak{C}_{\text{ext}}$*-equivalent to* φ_h^{ext} *has size* $> \text{Tower}(h{+}3)$*, and*

(3) φ_h^{ext} *is preserved under extensions on* $\mathfrak{C}_{\text{ext}}$*.*

Proof. Recall that each extension of a structure $\mathcal{A}$ contains $\mathcal{A}$ as an *induced* substructure. Consider a complete ordered binary tree $\mathcal{A} \in \mathfrak{C}_{\text{ext}}$ of height $n \geq 1$ and let a be its root node. Assume that $\mathcal{S}^{\Theta^{\text{ext}}[\mathcal{A}]}(a)$ is a binary tree of height at most $n-1$. Then, every leaf b of $\mathcal{S}^{\Theta^{\text{ext}}[\mathcal{A}]}(a)$ has an S_0-successor and an S_1-successor in $\mathcal{A}$ but is neither contained in $L_0^{\mathcal{A}}$ nor in $L_1^{\mathcal{A}}$. Therefore, for each extension $\mathcal{B}$ of $\mathcal{A}$ from $\mathfrak{C}_{\text{ext}}$ we have that $\mathcal{S}^{\Theta^{\text{ext}}[\mathcal{A}]}(a)$ and $\mathcal{S}^{\Theta^{\text{ext}}[\mathcal{B}]}(a)$ are isomorphic.

We will use the latter observation to protect binary tree encodings, embedded in ordered binary trees from $\mathfrak{C}_{\text{ext}}$, against modifications by extensions to the underlying ordered binary tree. Towards this aim, recall that we know by Lemma 9.6.6 that for each $h > 1$ and every $i \in [0, \text{Tower}(h{+}3))$, each binary tree in $\mathfrak{B}_h(i)$ has height $< 2 \cdot \text{Tower}(h{+}1)$.

Similar to the $\mathsf{FO}[E]$-formula $\text{complete}_n(x)$ defined in the proof of Lemma 9.6.4, we can define an $\mathsf{FO}[\sigma_{\text{ext}}]$-formula $\text{complete}'_n(x)$ of size $\log(n)$ for $n \geq 1$ that is satisfied by a node a in an ordered binary forest $\mathcal{A}$ from $\mathfrak{C}_{\text{ext}}$ or $\mathfrak{C}_{\text{hom}}$ if and only if $\mathcal{S}_n^{\mathcal{A}}(a)$ is complete with height n.

In the following, we aim to transform Sentence (9.1), for each $h > 1$, into an $\mathsf{FO}[\sigma_{\text{ext}}]$-sentence that not only has large $\mathfrak{C}_{\text{ext}}$-minimal models but that is also preserved under extensions on $\mathfrak{C}_{\text{ext}}$. To this end, we use the Θ^{ext}-reducts of the $\mathsf{FO}[E]$-formulae of Lemma 9.6.4 and Lemma 9.6.5.

For each $h > 1$, we let

$$\begin{aligned}
\varphi_h^{\text{ext}} \;\; \coloneqq \;\; & \exists x \left(\text{enc}_h^{\text{ext}}(x) \;\wedge\; \min_h^{-\Theta^{\text{ext}}}(x)\right) \;\;\wedge \\
& \forall x \Biggl(\text{enc}_h^{\text{ext}}(x) \;\rightarrow \\
& \qquad \left(\max_h^{-\Theta^{\text{ext}}}(x) \;\vee\; \exists y \left(\text{enc}_h^{\text{ext}}(y) \;\wedge\; \text{succ}_h^{-\Theta^{\text{ext}}}(x,y)\right)\right)\Biggr)
\end{aligned}$$

with

$$\text{enc}_h^{\text{ext}}(x) \;\coloneqq\; \text{enc}_h^{-\Theta^{\text{ext}}}(x) \;\wedge\; \text{complete}'_{2\cdot\text{Tower}(h+1)}(x).$$

For the fixed transduction Θ^{ext} it follows from Lemma 2.6.4 that for each formula φ from $\mathsf{FO}[E]$, the size of the Θ^{ext}-reduct $\varphi^{-\Theta^{\text{ext}}}$ is linear in the size of φ.

Therefore, by Lemma 9.6.4 and Lemma 9.6.5, and since $\mathrm{complete}'_{2\cdot\mathrm{Tower}(h+1)}(x)$ has size in $\mathcal{O}(\mathrm{Tower}(h))$, the following claim holds.

Claim 1. *There is a $c \in \mathbb{N}_{\geq 1}$ such that $||\varphi_h^{\mathrm{ext}}|| \leq c \cdot \mathrm{Tower}(h)$ for each $h > 1$.*

For the following, we fix a number $h > 1$. The proof of Lemma 9.6.7 is completed by showing the following to claims.

Claim 2. *Every existential $\mathsf{FO}[\sigma_{\mathrm{ext}}]$-sentence that is $\mathfrak{C}_{\mathrm{ext}}$-equivalent to φ_h^{ext} has size $>$ $\mathrm{Tower}(h{+}3)$.*

Proof of Claim 2. It is straightforward to see that there are structures in $\mathfrak{C}_{\mathrm{ext}}$ that satisfy φ_h^{ext}. In particular, by definition of the subformulae of φ_h^{ext} in Lemma 9.6.4 and Lemma 9.6.5, each model $\mathcal{A} \in \mathfrak{C}_{\mathrm{ext}}$ of φ_h^{ext} has to contain at least a number of $\mathrm{Tower}(h{+}3)$ pairwise distinct nodes $a_0, \ldots, a_{\mathrm{Tower}(h+3)-1}$ such that, for each $i \in [0, \mathrm{Tower}(h{+}3))$, $\mathcal{S}^{\Theta^{\mathrm{ext}}[\mathcal{A}]}(a_i) \in \mathfrak{B}_h(i)$, that is, $\mathcal{S}^{\Theta^{\mathrm{ext}}[\mathcal{A}]}(a_i)$ is a binary tree encoding of the number i with parameter h. Thus, since $\mathfrak{C}_{\mathrm{ext}}$ is closed under induced substructures, Claim 2 follows from Lemma 9.6.3.

Claim 3. *φ_h^{ext} is preserved under extensions on $\mathfrak{C}_{\mathrm{ext}}$.*

Proof of Claim 3. Consider a model $\mathcal{A} \in \mathfrak{C}_{\mathrm{ext}}$ of φ_h^{ext}. By construction of the sentence φ_h^{ext}, there are pairwise distinct nodes $a_0, \ldots, a_{\mathrm{Tower}(h+3)-1}$ in $\mathcal{A}$ such that, for each $i \in [0, \mathrm{Tower}(h{+}3))$, $\mathcal{S}^{\Theta^{\mathrm{ext}}[\mathcal{A}]}(a_i)$ belongs to the set $\mathfrak{B}_h(i)$ and, in particular, has height $< 2 \cdot \mathrm{Tower}(h{+}1)$.

Let $\mathcal{B} \in \mathfrak{C}_{\mathrm{ext}}$ be an extension of $\mathcal{A}$. By construction of the subformula $\mathrm{enc}_h^{\mathrm{ext}}(x)$ of φ_h^{ext}, for each $i \in [0, \mathrm{Tower}(h{+}3))$, the substructure $\mathcal{S}^{\mathcal{A}}_{2\cdot\mathrm{Tower}(h+1)}(a_i)$ is a complete ordered binary tree of height $2 \cdot \mathrm{Tower}(h{+}1)$. Therefore, $\mathcal{S}^{\Theta^{\mathrm{ext}}[\mathcal{A}]}(a_i)$ and $\mathcal{S}^{\Theta^{\mathrm{ext}}[\mathcal{B}]}(a_i)$ are isomorphic and thus, also $\mathcal{S}^{\Theta^{\mathrm{ext}}[\mathcal{B}]}(a_i)$ belongs to the set $\mathfrak{B}_h(i)$. On the other hand, let b be a node from $\mathcal{B}$ such that $\mathcal{B} \models \mathrm{enc}_h^{\mathrm{ext}}[b]$. Then, there is an $i \in [0, \mathrm{Tower}(h{+}3))$ such that $\mathcal{S}^{\Theta^{\mathrm{ext}}[\mathcal{B}]}(b)$ belongs to $\mathfrak{B}_h(i)$ and hence, either $\mathcal{B} \models \mathrm{max}_h^{-\Theta^{\mathrm{ext}}}[b]$ or $\mathcal{B} \models \mathrm{succ}_h^{-\Theta^{\mathrm{ext}}}[b, a_{i+1}]$. In both cases, $\mathcal{B} \models \varphi_h^{\mathrm{ext}}$.

This completes the proof of Claim 3 and thus also the proof of Lemma 9.6.7. □

9.6.3 Preservation under Homomorphisms

This section is devoted to the proof of Theorem 9.6.2. Here, we need to construct $\mathsf{FO}[\sigma_{\mathrm{hom}}]$-sentences with large $\mathfrak{C}_{\mathrm{hom}}$-minimal models that are preserved under homomorphism on $\mathfrak{C}_{\mathrm{hom}}$. Recall that σ_{hom} is the signature consisting of the binary relation symbols S_0 and S_1, and a unary relation symbol L_M for each $M \subseteq \{0, 1\}$.

Furthermore, recall that in any $\mathcal{A} \in \mathfrak{C}_{\text{hom}}$, each node belongs to precisely one of the unary relations $L_M^{\mathcal{A}}, M \subseteq \{0,1\}$. In other words, $L_M^{\mathcal{A}}$, $M \subseteq \{0,1\}$ are a colouring of the nodes of $\mathcal{A}$. In particular, this implies that, if there is a homomorphism h from $\mathcal{A}$ to a structure $\mathcal{B} \in \mathfrak{C}_{\text{hom}}$, then

$$a \in L_M^{\mathcal{A}} \quad \text{iff} \quad h(a) \in L_M^{\mathcal{B}} \quad \text{for all } a \in A \text{ and } M \subseteq \{0,1\}. \tag{9.2}$$

In the following, we embed binary forest from $\mathfrak{BF}$ in complete ordered binary trees from $\mathfrak{C}_{\text{hom}}$. Similar to Section 9.6.2, we describe this embedding as a transduction $\Theta^{\text{hom}} := (\theta^{\text{hom}}, \theta_E^{\text{hom}})$ from σ_{hom} to (E), defined by $\theta^{\text{hom}}(x) := x{=}x$ and

$$\theta_E^{\text{hom}}(x,y) \;:=\; \bigvee_{i\in\{0,1\}} \Bigg(S_i(x,y) \;\; \wedge \bigvee_{\substack{M\subseteq\{0,1\},\\ i\in M}} L_M(x) \Bigg).$$

Thus, for every ordered binary forest $\mathcal{A}$ from $\mathfrak{C}_{\text{hom}}$, $\Theta^{\text{hom}}[\mathcal{A}]$ is the unordered binary forest from $\mathfrak{BF}$ which contains the same nodes as $\mathcal{A}$ and for all nodes $a, b \in A$, there is an edge from a to b if there is an $i \in \{0,1\}$ such that $(a,b) \in S_i^{\mathcal{A}}$ and $a \in L_M^{\mathcal{A}}$ for an $M \subseteq \{0,1\}$ with $i \in M$. Intuitively, the unique $M \subseteq \{0,1\}$ for which $a \in L_M^{\mathcal{A}}$ tells us whether an edge from a to a node b in the successor relations $S_0^{\mathcal{A}}$ and $S_1^{\mathcal{A}}$ is also an edge in $\Theta^{\text{hom}}[\mathcal{A}]$.

Note that we can interpret Figure 9.4 also as an illustration for the embedding described here. The only difference is that we have to understand the labelling of the nodes as an indicator for which unique unary relation $L_M^{\mathcal{A}}$ the node belongs to. That is, all unlabelled nodes belong to $L_\emptyset^{\mathcal{A}}$, all nodes labelled with 0 and 1 belong to $L_{\{0,1\}}^{\mathcal{A}}$, and all nodes labelled with 0 or 1 belong to $L_{\{0\}}^{\mathcal{A}}$ or $L_{\{1\}}^{\mathcal{A}}$, respectively.

Theorem 9.6.2 follows directly from Corollary 9.2.10 and the following lemma.

Lemma 9.6.8. *There is a number $c \in \mathbb{N}_{\geq 1}$ and a sequence $(\varphi_h^{\text{hom}})_{h>1}$ of sentences from $\mathsf{FO}[\sigma_{\text{hom}}]$ such that for each $h > 1$,*

(1) $||\varphi_h^{\text{hom}}|| \leq c \cdot \text{Tower}(h)$*,*

(2) every existential-positive $\mathsf{FO}[\sigma_{\text{hom}}]$-sentence that is $\mathfrak{C}_{\text{hom}}$-equivalent to φ_h^{hom} has size $>$ $\text{Tower}(h{+}3)$, and

(3) φ_h^{hom} is preserved under homomorphisms on $\mathfrak{C}_{\text{hom}}$.

Proof. Consider a complete ordered binary tree $\mathcal{A} \in \mathfrak{C}_{\text{hom}}$ with height $n \geq 1$ and let a its root node. Observe that every homomorphism h from $\mathcal{A}$ to an ordered binary forest $\mathcal{B} \in \mathfrak{C}_{\text{hom}}$ is injective. Furthermore, if $\mathcal{S}^{\Theta^{\text{hom}}[\mathcal{A}]}(a)$ is a binary tree of height at most $n-1$, then $\mathcal{S}^{\Theta^{\text{hom}}[\mathcal{A}]}(a)$ and $\mathcal{S}^{\Theta^{\text{hom}}[\mathcal{B}]}(h(a))$ are isomorphic.

The remainder of the proof is very similar to the one of Lemma 9.6.7. We define a sequence $(\varphi_h^{\text{hom}})_{h>1}$ of $\mathsf{FO}[\sigma_{\text{hom}}]$-sentences in the same way as the sequence $(\varphi_h^{\text{ext}})_{h>1}$ in the proof of Lemma 9.6.7, with the only difference being that we use reducts in respect to the transduction Θ^{hom} instead of the transduction Θ^{ext}. That is, for each $h > 1$, we let

$$\begin{aligned}\varphi_h^{\text{hom}} \;:=\;\; & \exists x \left(\text{enc}_h^{\text{hom}}(x) \;\wedge\; \min_h^{-\Theta^{\text{hom}}}(x)\right) \;\wedge \\ & \forall x \Bigg(\text{enc}_h^{\text{hom}}(x) \;\to \\ & \qquad \left(\max_h^{-\Theta^{\text{hom}}}(x) \;\vee\; \exists y \left(\text{enc}_h^{\text{hom}}(y) \;\wedge\; \text{succ}_h^{-\Theta^{\text{hom}}}(x,y)\right)\right)\Bigg)\end{aligned}$$

with

$$\text{enc}_h^{\text{hom}}(x) \;:=\; \text{enc}_h^{-\Theta^{\text{hom}}}(x) \;\wedge\; \text{complete}'_{2\cdot\text{Tower}(h+1)}(x).$$

By this construction, we immediately obtain that Statement (1) holds

Let $h > 1$. In an analogous way to Claim 2 in the proof of Lemma 9.6.7, we obtain that each model of φ_h^{hom} from $\mathfrak{C}_{\text{hom}}$, has a universe of size at least $\text{Tower}(h{+}3)$. Since every existential-positive sentence is, in particular, an existential sentence and since $\mathfrak{C}_{\text{hom}}$ is closed under induced substructures, we obtain Statement (2) from Lemma 9.6.3.

To show that φ_h^{hom} *is preserved under extensions on* $\mathfrak{C}_{\text{hom}}$ and thus, Statement (3) is satisfied, we also can proceed in a similar fashion as in the proof of Lemma 9.6.7. Consider a model $\mathcal{A} \in \mathfrak{C}_{\text{hom}}$ of φ_h^{hom}. By construction of φ_h^{hom}, there are pairwise distinct nodes $a_0, \ldots, a_{\text{Tower}(h+3)-1}$ in $\mathcal{A}$ such that, for each $i \in [0, \text{Tower}(h{+}3))$, $\mathcal{S}^{\Theta^{\text{hom}}[\mathcal{A}]}(a_i)$ belongs to the set $\mathfrak{B}_h(i)$ and thus has height $< 2 \cdot \text{Tower}(h{+}1)$.

Let $\mathcal{B} \in \mathfrak{C}_{\text{hom}}$ such that there is a homomorphism h from $\mathcal{A}$ to $\mathcal{B}$. By construction of the subformula $\text{enc}_h^{\text{hom}}(x)$ of φ_h^{hom}, for each $i \in [0, \text{Tower}(h{+}3))$, the substructure $\mathcal{S}^{\mathcal{A}}_{2\cdot\text{Tower}(h+1)}(a_i)$ is a complete ordered binary tree of height $2 \cdot \text{Tower}(h{+}1)$. Therefore, $\mathcal{S}^{\Theta^{\text{hom}}[\mathcal{A}]}(a_i)$ and $\mathcal{S}^{\Theta^{\text{hom}}[\mathcal{B}]}_{h(a_i)}$ are isomorphic and thus, also $\mathcal{S}^{\Theta^{\text{hom}}[\mathcal{B}]}(h(a_i))$ belongs to the set $\mathfrak{B}_h(i)$. On the other hand, let b be a node from $\mathcal{B}$ such that $\mathcal{B} \models \text{enc}_h^{\text{hom}}[b]$. Then, there is an $i \in [0, \text{Tower}(h{+}3))$ such that $\mathcal{S}^{\Theta^{\text{hom}}[\mathcal{B}]}(b)$ belongs to $\mathfrak{B}_h(i)$ and hence, either $\mathcal{B} \models \max_h^{-\Theta^{\text{hom}}}[b]$ or $\mathcal{B} \models \text{succ}_h^{-\Theta^{\text{hom}}}[b, h(a_{i+1})]$. We can conclude that $\mathcal{B} \models \varphi_h^{\text{hom}}$.

This completes the proof of Lemma 9.6.8. □

9.7 Conclusion

In this chapter, we have proven lower bounds for the time complexity of the algorithms presented in the previous chapters. While most of these algorithms were generalised to extensions of first-order logic by ultimately periodic counting quantifiers that were even allowed to count tuples, all lower bounds already hold for plain first-order logic FO.

For the construction of Hanf normal form, Gaifman normal form, and Feferman-Vaught decompositions, the lower bounds are 3-fold exponential in the size of the input formula for degree bounds $d \geq 3$, and 2-fold exponential for $d = 2$, showing that our corresponding algorithms are basically worst-case optimal.

For the construction of existential sentences for sentences that are preserved under extensions on structures of degree $d \geq 3$, we have proven a non-matching 3-fold exponential lower bound. The same holds for the construction of existential-positive sentences for sentences that are preserved under extensions.

All lower bounds rely on encodings of large initial segments of the natural numbers by tree-like structures of bounded degree that can be compared by small formulae. In particular, for Hanf normal form, Gaifman normal form, and Feferman-Vaught decompositions, the combinatorial essence of the proofs was stated in such a way that it can be applied to various classes of structures.

10 Conclusion

This chapter concludes the thesis with a short summary of its main results and some directions for further research. The aim of this thesis was to investigate the complexity of normal forms for (extensions of) first-order logic on classes of structures of bounded degree. This was motivated by the fact that, already on classes of acyclic structures without degree limit, normal forms like Gaifman normal form [Gai82], Feferman-Vaught decompositions [FV59], and existential(-positive) formulae for formulae that are preserved under extensions (homomorphisms) (cf., e.g., [Lyn59, Hod93, Ros08]), have a non-elementary blow-up [DGKS07, Ros08]. The main results of this thesis are, contrary to this, elementary and, for Gaifman normal form and Feferman-Vaught decompositions, worst-case optimal algorithms for classes of structures of bounded degree.

In another direction, extensions of first-order logic (FO) by sets of unary counting quantifiers are characterised that permit suitable generalisations of Hanf normal form [BK12]. It turns out that these are precisely sets of ultimately periodic quantifiers. For the respective extensions of FO, it was shown that Hanf normal form can be computed in worst-case optimal time. In particular, this led to corresponding generalisations of the aforementioned algorithms for Feferman-Vaught decompositions and preservation theorems. Furthermore, following a well-known construction (described, e.g., in [Str94]), these algorithms could even be extended to formulae with tuple-counting quantifiers.

This thesis' results were largely published in [HKS13, HHS14, HHS15, HKS16].

In the following, we fix a degree bound $d \geq 2$, let $\mathfrak{C}_d$ denote the class of all d-bounded structures over a relational signature σ, and restrict attention to formulae over this signature.

Results for First-Order Logic

Let us first focus on the special case of FO. This thesis' main results concerning Gaifman normal form and Feferman-Vaught decompositions can be stated as follows:

(G) For each formula φ of $\mathsf{FO}[\sigma]$, a d-equivalent Gaifman normal form can be constructed in 3-fold (2-fold) exponential time for $d \geq 3$ ($d = 2$).

(FV) For each formula φ of $\mathsf{FO}[\sigma_s]$, for $s \geq 1$, a decomposition with respect to s-ary disjoint sums of structures from $\mathfrak{C}_d$ can be constructed in 3-fold (2-fold) exponential time for $d \geq 3$ ($d = 2$).

The latter result (FV) was, moreover, adapted to decompositions with respect to direct products and, more generally, decompositions with respect to transductions over disjoint sums. For (G) as well as for (FV) matching lower bounds were shown, implying the worst-case optimality of both algorithms. The construction for Gaifman normal form (G) and the matching lower bound are based on [HKS13], while (FV) and the corresponding matching lower bound are based on [HHS14, HHS15]. In both algorithms, the first step is the construction of a d-equivalent Hanf normal form. This is followed by a transformation of the sphere-formulae and counting-sentences in the Hanf normal form, which is irrespective of the degree bound.

Concerning the preservation theorems of Lyndon, Łoś, and Tarski, this thesis provides the following results:

(PE) For each formula φ of $\mathsf{FO}[\sigma]$ that is preserved under extensions on $\mathfrak{C}_d$, a d-equivalent existential $\mathsf{FO}[\sigma]$-formula can be constructed in 5-fold (3-fold) exponential time for $d \geq 3$ ($d = 2$).

(PH) For each formula φ of $\mathsf{FO}[\sigma]$ that is preserved under homomorphisms on $\mathfrak{C}_d$, a d-equivalent existential-positive $\mathsf{FO}[\sigma]$-formula can be constructed in 4-fold (3-fold) exponential time for $d \geq 3$ ($d = 2$).

Note that (PE) and (PH) do not only hold on the class $\mathfrak{C}_d$, but on all classes of d-bounded σ-structures that are closed under disjoint unions and induced substructures and that, for (PH), are decidable in 1-fold exponential time. Furthermore, both closure properties were actually shown to be unavoidable. The upper bounds of (PE) and (PH) are complemented by (non-matching) 3-fold exponential lower bounds. (PE) and (PH), as well as counterexamples for the closure properties and the lower bounds, were first published in [HHS14, HHS15]. There, both results already extend to FO-sentences with one modulo-counting quantifier, but only consider formulae without free variables.

The crucial ingredient in both algorithms is an upper bound on the size of $\mathfrak{C}_d$-minimal models for the input formula, which is obtained by using Hanf's

	$d \geq 3$	$d = 2$
Hanf normal form	3-exp	2-exp
Gaifman normal form	3-exp	2-exp
Feferman-Vaught decompositions	3-exp	2-exp
Preservation under extensions	5-exp	3-exp
Preservation under homomorphisms	4-exp	3-exp

Figure 10.1 Overview over the runtime of the normal form algorithms on $\mathfrak{C}_d$. Here, k-exp means that the algorithm has k-fold exponential time complexity in respect to the size of the input formula. For the results concerning Hanf normal form, Gaifman normal form, and Feferman-Vaught decompositions, matching lower bounds for $d \geq 3$ and $d = 2$ were proven. For the results concerning preservation theorems, 3-fold exponential lower bounds for $d = 3$ were shown. For extensions of FO by ultimately periodic quantifiers, the algorithms for Hanf normal form, Feferman-Vaught decompositions, and preservation theorems have roughly the same time complexity.

locality theorem. In the case of (PE), this requires a novel iterative construction, whereas for (PH), a proof in [AG94], which originally uses Gaifman's theorem, is adapted.

Extensions of First-Order Logic

A crucial tool for the aforementioned results are Hanf's locality theorem [Han65, FSV95] and the corresponding Hanf normal form [BK12] which, in its own right, is an important ingredient for algorithms on classes of structures of bounded degree [See96, FG04, DG07, KS11, BKS17, KS17]. The observation that locality theorems in the manner of Hanf's theorem do not only hold for FO but also for certain extensions of FO by additional quantifiers [Nur00], opened a second line of research of this thesis. There, it was asked which extensions of FO by unary counting quantifiers also permit Hanf normal form and, if yes, how to compute this Hanf normal form effectively. Answering the first question about a characterisation of logics permitting Hanf normal form, it was shown that:

(HC) An extension of FO by unary counting quantifiers permits Hanf normal form if and only if all its quantifiers are ultimately periodic.

In particular, this includes the extensions of FO by threshold-counting and modulo-counting quantifiers. Furthermore, by using a well-known construction (cf. [Str94]), it also includes extensions of FO by ultimately periodic counting quantifiers that are allowed to count over tuples of elements instead of single elements of structures.

To show that ultimately periodic quantifiers permit Hanf normal form, we first generalised the algorithm of [BK12] to extensions of FO by modulo-counting quantifiers. In a second step, we have expressed ultimately periodic quantifiers by modulo-counting quantifiers and vice versa. On the other hand, even a very simple sentence over the signature (P), where P is a unary relation symbol, stating that the cardinality of a structure belongs to a set that is not ultimately periodic, can not be expressed by a Hanf normal form.

The second result in this direction shows that, if an extension of FO by unary counting quantifiers permits Hanf normal form, then such Hanf normal forms can also be computed efficiently:

(HA) For each extension of FO that permits Hanf normal form, every formula φ can be turned into a d-equivalent Hanf normal form in 3-fold (2-fold) exponential time for $d \geq 3$ ($d = 2$).

This algorithm follows directly from an analysis of the proof of (HC). Matching lower bounds, already presented in [BK12], show the worst-case optimality of the algorithm implied by (HA). As an application, (HA) leads to straightforward extensions of Seese's fixed-parameter model-checking algorithm on $\mathfrak{C}_d$ [See96] for formulae with ultimately periodic quantifiers.

Moreover, (HC) and (HA) allow the generalisation of the results (FV), (PE), and (PH) to extensions of FO by ultimately periodic quantifiers. In all these cases, we obtain algorithms with basically the same time complexity as in the case of FO, which are therefore worst-case optimal. For the case of Feferman-Vaught decompositions, it was proven that a similar characterisation as (HC) holds:

(FVC) An extension of FO by unary counting quantifiers permits decompositions with respect to disjoint sums if and only if all its quantifiers are ultimately periodic.

(HC) as well as (HA) were first published in [HKS16], although without regard to tuple-quantifiers. The variants of (PE) and (PH) for the case of FO with an additional modulo-counting quantifier were published in [HHS14, HHS15].

Note that recently it was shown in [KS17] that a weaker variant of Hanf normal form, where counting-sentences may count over disjunctions of types, can be constructed for arbitrary sets of unary counting quantifiers and not only for ultimately periodic quantifiers.

For Gaifman normal form, [KS18] presents a generalisation to extensions of FO by unary counting quantifiers and shows that (on all structures) equivalent formulae in Gaifman normal form can be computed if and ony if all quantifiers involved are ultimately periodic. This is used in [KS18] to extend a result of [FG01] in order to show the fixed-parameter tractability of the model-checking problem for such logics on classes of structures of bounded local tree-width. For classes of structures of bounded degree, [KS18] shows that Gaifman normal form exists even for arbitrary unary counting quantifiers and can be constructed in worst-case optimal 3-fold exponential time if all quantifiers involved are ultimately periodic.

Further Research

The results of this thesis are stated for the setting of finite structures. One aim would be to determine which of these results also hold for infinite structures.

For applications of Hanf normal form in model-checking and related tasks, a possible direction of further research would be to examine constructions of Hanf normal form which are guided by the specific task, e.g., by only performing a partial construction of the Hanf normal form with respect to a fixed structure.

Concerning preservation theorems, an obvious direction of further research is to close the gap between the upper and the lower bounds provided in this thesis. For (PE), there might be potential for finding a better upper bound on the size of minimal models. For (PH), an alternative to the Chandra-Merlin theorem [CM77, AHV95], e.g., in a similar way to the relativisation of quantifiers used for (PE), could lead to a better upper bound.

Similarly to the Łoś-Tarski-theorem, Lyndon's positivity theorem [Lyn59], stating that an FO-sentence is preserved under surjective homomorphisms if and only if it is equivalent to a positive sentence, is known to fail on finite structures [AG87, Sto95]. To the author's knowledge, it is not known whether there are classes of finite structures for which it can be reestablished. It would be interesting to identify such classes and then, to examine the complexity of constructing the positive sentences with respect to these classes.

Finally, besides Gaifman normal form and Hanf normal form, there is a further local normal form, described in [SB99], that invites an investigation into its efficiency.

Bibliography

[ADG08] Albert Atserias, Anuj Dawar, and Martin Grohe. Preservation under extensions on well-behaved finite structures. *SIAM Journal on Computing*, 38(4):1364–1381, 2008.

[ADK06] Albert Atserias, Anuj Dawar, and Phokion G. Kolaitis. On preservation under homomorphisms and unions of conjunctive queries. *Journal of the ACM*, 53(2):208–237, 2006.

[AG87] Miklós Ajtai and Yuri Gurevich. Monotone versus positive. *Journal of the ACM*, 34(4):1004–1015, 1987.

[AG94] Miklós Ajtai and Yuri Gurevich. Datalog vs first-order logic. *Journal of Computer and System Sciences*, 49(3):562–588, 1994.

[AHV95] Serge Abiteboul, Richard Hull, and Victor Vianu, editors. *Foundations of Databases: The Logical Level.* Addison-Wesley Longman Publishing Co., Inc., Boston, MA, USA, 1st edition, 1995.

[BK12] Benedikt Bollig and Dietrich Kuske. An optimal construction of Hanf sentences. *Journal of Applied Logic*, 10(2):179–186, 2012.

[BKS17] Christoph Berkholz, Jens Keppeler, and Nicole Schweikardt. Answering FO+MOD queries under updates on bounded degree databases. In Michael Benedikt and Giorgio Orsi, editors, *20th International Conference on Database Theory (ICDT 2017)*, volume 68 of *Leibniz International Proceedings in Informatics (LIPIcs)*, pages 8:1–8:18, Dagstuhl, Germany, 2017. Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik.

[Clo12] Martin Clochard. Énumération de requêtes du premier ordre sur les structures de degré borné, 2012. Report on internship at Équipe de Logique Mathématique Université Denis-Diderot Paris 7, supervised by Arnaud Durand.

[CM77] Ashok K. Chandra and Philip M. Merlin. Optimal implementation of conjunctive queries in relational data bases. In *Proceedings of the 9th Annual ACM Symposium on Theory of Computing, STOC'77*, pages 77–90, 1977.

[Daw10] Anuj Dawar. Homomorphism preservation on quasi-wide classes. *Journal of Computer and System Sciences*, 76(5):324–332, 2010.

[DG07] Arnaud Durand and Etienne Grandjean. First-order queries on structures of bounded degree are computable with constant delay. *ACM Transactions on Computational Logic*, 8(4), 2007.

[DGKS06] Anuj Dawar, Martin Grohe, Stephan Kreutzer, and Nicole Schweikardt. Approximation schemes for first-order definable optimisation problems. In *Proceedings of the 21th Annual IEEE Symposium on Logic in Computer Science (LICS 2006)*, pages 411–420, 2006.

[DGKS07] Anuj Dawar, Martin Grohe, Stephan Kreutzer, and Nicole Schweikardt. Model Theory Makes Formulas Large. In *Proceedings of the 34th International Colloquium on Automata, Languages and Programming (ICALP 2007)*, pages 1076–1088, 2007. Full version available as preprint NI07003-LAA, Isaac Newton Institute of Mathematical Sciences (2007).

[DSS14] Arnaud Durand, Nicole Schweikardt, and Luc Segoufin. Enumerating Answers to First-Order Queries over Databases of Low Degree. In *Proceedings of the 33th ACM SIGMOD/PODS Symposium on Principles of Database Systems (PODS 2014)*, Snowbird, USA, 2014.

[EF99] Heinz-Dieter Ebbinghaus and Jörg Flum. *Finite Model Theory.* Springer, 1999.

[FG01] Markus Frick and Martin Grohe. Deciding first-order properties of locally tree-decomposable structures. *Journal of the ACM*, 48(6):1184–1206, 2001.

[FG04] Markus Frick and Martin Grohe. The complexity of first-order and monadic second-order logic revisited. *Annals of Pure and Applied Logic*, 130(1-3):3–31, 2004.

[FG06] Jörg Flum and Martin Grohe. *Parameterized Complexity Theory*. Springer-Verlag Berlin Heidelberg, 2006.

[FSV95] Ronald Fagin, Larry J. Stockmeyer, and Moshe Y. Vardi. On monadic NP vs. monadic co-NP. *Information and Computation*, 120(1):78–92, 1995.

[FV59] Solomon Feferman and Robert L. Vaught. The first order properties of products of algebraic systems. *Fundamenta Mathematicae*, 47:57–103, 1959.

[Gai82] Haim Gaifman. On local and non-local properties. In J. Stern, editor, *Proceedings of the Herbrand Symposium, Logic Colloquium '81*, pages 105–135. North Holland, 1982.

[GJL12] Stefan Göller, Jean Christoph Jung, and Markus Lohrey. The complexity of decomposing modal and first-order theories. In *Proceedings of the 27th Annual IEEE Symposium on Logic in Computer Science (LICS 2012)*, pages 325–334, 2012.

[GKS14] Martin Grohe, Stephan Kreutzer, and Sebastian Siebertz. Deciding first-order properties of nowhere dense graphs. In David B. Shmoys, editor, *Symposium on Theory of Computing, STOC 2014, New York, NY, USA, May 31 - June 03, 2014*, pages 89–98. ACM, 2014.

[Gro17] Martin Grohe. *Descriptive Complexity, Canonisation, and Definable Graph Structure Theory*. Lecture Notes in Logic. Cambridge University Press, 2017. To appear. Preliminary version available at `https://www.lii.rwth-aachen.de/de/13-mitarbeiter/professoren/39-book-descriptive-complexity.html`.

[Gru16] Berit Grußien. *Capturing Polynomial Time and Logarithmic Space using Modular Decompositions and Limited Recursion*. PhD thesis, Department of Computer Science, Humboldt-Universität zu Berlin, 2016.

[GS04] Martin Grohe and Nicole Schweikardt. Comparing the succinctness of monadic query languages over finite trees. *RAIRO - Theoretical Informatics and Applications*, 38(4):343–373, 2004.

[GS05] Martin Grohe and Nicole Schweikardt. The succinctness of first-order logic on linear orders. *Logical Methods in Computer Science*, 1(1), 2005.

[Gur84] Yuri Gurevich. Toward logic tailored for computational complexity. In M. Richter et al., editor, *Computation and Proof Theory*, volume 1104 of *Lecture Notes in Mathematics*, pages 175–216. Springer, 1984.

[Gur90] Yuri Gurevich. *On Finite Model Theory (Extended Abstract)*, pages 211–219. Birkhäuser Boston, Boston, MA, 1990.

[GW04] Martin Grohe and Stefan Wöhrle. An existential locality theorem. *Annals of Pure and Applied Logic*, 129(1-3):131–148, 2004.

[Han65] William Hanf. Model-theoretic methods in the study of elementary logic. In J.W. Addison, L. Henkin, and A. Tarski, editors, *The Theory of Models*, pages 132–145. North Holland, 1965.

[Hei12] Lucas Heimberg. Gaifman-Normalformen auf Strukturklassen beschränkten Grades. Diplomarbeit, HU Berlin, 2012.

[HHS14] Frederik Harwath, Lucas Heimberg, and Nicole Schweikardt. Preservation and decomposition theorems for bounded degree structures. In *Joint Meeting of the 23rd EACSL Annual Conference on Computer Science Logic (CSL) and the 29th Annual ACM/IEEE Symposium on Logic in Computer Science (LICS), (CSL-LICS 2014)*, pages 49:1–49:10. ACM, 2014.

[HHS15] Frederik Harwath, Lucas Heimberg, and Nicole Schweikardt. Preservation and decomposition theorems for bounded degree structures. *Logical Methods in Computer Science*, 11(4), 2015.

[HKS13] Lucas Heimberg, Dietrich Kuske, and Nicole Schweikardt. An optimal Gaifman normal form construction for structures of bounded degree. In *Proceedings of the 28th Annual ACM/IEEE Symposium on Logic in Computer Science, (LICS 2013)*, pages 63–72, 2013.

[HKS16] Lucas Heimberg, Dietrich Kuske, and Nicole Schweikardt. Hanf normal form for first-order logic with unary counting quantifiers. In *Proceedings of the 31th Annual ACM/IEEE Symposium on Logic in Computer Science, (LICS 2016)*, pages 63–72, 2016.

[HLN99] Lauri Hella, Leonid Libkin, and Juha Nurmonen. Notions of locality and their logical characterizations over finite models. *Journal of Symbolic Logic*, 64(4):1751–1773, 1999.

[Hod93] Wilfrid Hodges. *Model Theory*. Cambridge University Press, 1993.

[KM14] Tomer Kotek and Johann A. Makowsky. Connection matrices and the definability of graph parameters. *Logical Methods in Computer Science*, 10(4), 2014.

[Kre11] Stephan Kreutzer. Algorithmic meta-theorems. In *Finite and Algorithmic Model Theory*. Cambridge University Press, 2011. London Mathematical Society Lecture Notes, No. 379.

[KS11] Wojciech Kazana and Luc Segoufin. First-order query evaluation on structures of bounded degree. *Logical Methods in Computer Science*, 7(2), 2011.

[KS17] Dietrich Kuske and Nicole Schweikardt. First-order logic with counting: At least, weak Hanf normal forms always exist and can be computed! In *Proceedings of the 32nd Annual ACM/IEEE Symposium on Logic in Computer Science, (LICS 2017)*, 2017. To appear. Full version available at `https://arxiv.org/abs/1703.01122`.

[KS18] Dietrich Kuske and Nicole Schweikardt. Gaifman normal forms for counting extensions of first-order logic. In *Proceedings of the 45th International Colloquium on Automata, Languages, and Programming (ICALP 2018)*, 2018. To appear.

[Lib97] Leonid Libkin. On the forms of locality over finite models. In *Proceedings of the 12th Annual IEEE Symposium on Logic in Computer Science (LICS 1997)*, pages 204–215, 1997.

[Lib98] Leonid Libkin. On counting logics and local properties. In *Proceedings of the 13th Annual IEEE Symposium on Logic in Computer Science*, LICS 1998, pages 501–, Washington, DC, USA, 1998. IEEE Computer Society.

[Lib04] Leonid Libkin. *Elements of Finite Model Theory*. Springer, 2004.

[Lin08] Steven Lindell. A normal form for first-order logic over doubly-linked data structures. *International Journal of Foundations of Computer Science*, 19(1):205–217, 2008.

[LN00] Leonid Libkin and Juha Nurmonen. Counting and locality over finite structures: A survey. In *Revised Lectures from the 9th European Summer School on Logic, Language, and Information: Generalized Quantifiers and Computation*, ESSLLI '97, pages 18–50, London, UK, UK, 2000. Springer-Verlag.

[Lot84] M. Lothaire. *Combinatorics on words.* Cambridge University Press, 1984.

[Lyn59] Roger C. Lyndon. Properties preserved under homomorphism. *Pacific Journal of Mathematics*, 9(1):143–154, 1959.

[Mak04] Johann A. Makowsky. Algorithmic uses of the Feferman-Vaught theorem. *Annals of Pure and Applied Logic*, 126(1-3):159–213, 2004.

[Mat94] Armando B. Matos. Periodic sets of integers. *Theoretical Computer Science*, 127(2):287–312, 1994.

[NSST15] Frank Neven, Nicole Schweikardt, Frédéric Servais, and Tony Tan. Distributed streaming with finite memory. In *Proc. 18th International Conference on Database Theory (ICDT 2015)*, pages 324–341, 2015. Full version available at `https://www.csie.ntu.edu.tw/~tonytan/research/2015-icdt-dstj.pdf`.

[Nur96] Juha Nurmonen. On winning strategies with unary quantifiers. *Journal of Logic and Computation*, 6:779–798, 1996.

[Nur00] Juha Nurmonen. Counting modulo quantifiers on finite structures. *Information and Computation*, 160(1–2):62–87, 2000.

[PV06] Guoqiang Pan and Moshe Y. Vardi. Fixed-parameter hierarchies inside PSPACE. In *21th IEEE Symposium on Logic in Computer Science (LICS 2006), 12-15 August 2006, Seattle, WA, USA, Proceedings*, pages 27–36. IEEE Computer Society, 2006.

[Ros08] Benjamin Rossman. Homomorphism preservation theorems. *Journal of the ACM*, 55(3), 2008.

[Ros16] Benjamin Rossman. An improved homomorphism preservation theorem from lower bounds in circuit complexity. *SIGLOG News*, 3(4):33–46, 2016.

[SB99] Thomas Schwentick and Klaus Barthelmann. Local normal forms for first-order logic with applications to games and automata. *Discrete Mathematics and Computer Science*, 3:109–124, 1999.

[See96] Detlef Seese. Linear time computable problems and first-order descriptions. *Mathematical Structures in Computer Science*, 6(6):505–526, 1996.

[Seg14] Luc Segoufin. A glimpse on constant delay enumeration (invited talk). In *Proceedings of the 31st International Symposium on Theoretical Aspects of Computer Science (STACS 2014)*, pages 13–27, 2014.

[SM73] Larry J. Stockmeyer and Albert R. Meyer. Word problems requiring exponential time (preliminary report). In *Proceedings of the Fifth Annual ACM Symposium on Theory of Computing*, STOC '73, pages 1–9, New York, NY, USA, 1973. ACM.

[Sto95] Alexei P. Stolboushkin. Finitely monotone properties. In *Proceedings, 10th Annual IEEE Symposium on Logic in Computer Science, San Diego, California, USA, June 26-29, 1995*, pages 324–330. IEEE Computer Society, 1995.

[Str94] Howard Straubing. *Finite Automata, Formal Logic, and Circuit Complexity*. Birkhauser Verlag, Basel, Switzerland, Switzerland, 1994.

[Tai59] William W. Tait. A counterexample to a conjecture of Scott and Suppes. *Journal of Symbolic Logic*, 24:15–16, 1959.

[Wil94] Ross Willard. Hereditary undecidability of some theories of finite structures. *Journal of Symbolic Logic*, 59(4):1254–1262, 1994.

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Erklärung

Ich erkläre hiermit, dass

- ich die vorliegende Dissertation

  Complexity of Normal Forms on Structures of Bounded Degree

  selbstständig und ohne unerlaubte Hilfe angefertigt habe;
- ich mich weder bereits anderwärts um einen Doktorgrad im mathematisch-naturwissenschaftlichen Bereich beworben habe, noch einen solchen besitze;
- mir die Promotionsordnung der Mathematisch-Naturwissenschaftlichen Fakultät der Humboldt-Universität zu Berlin vom 30. Juni 2014, veröffentlicht im Amtlichen Mitteilungsblatt Nr. 126/2014, bekannt ist.

Berlin, den 4. 4. 2017

Lucas Heimberg